

in nodes :
 17 37 38 39 40 42 43 45 46 47 48 49 56 63 65 67 68 70 71 72 73 74 75
 76 77 79 80 81 82 84 85 86 88 89 91 92 93 95 96 97 98

g nodes :
 1 2 3 4 5 6 8 9 10 11 12 13 14 15 16 19 20 21 22 23 25 26 27 28 29
 31 32 33 34 35 51 52 53 54 55 58 59 60 61 62

n bonds :
 2-68 3-65 4-67 9-13 11-72 12-71 14-70 15-73 16-17 17-84 37-38 37-39 39-40
 42-43 42-45 46-47 46-48 48-49 53-56 60-63 74-75 75-76 75-77 79-80 80-81 81-82
 85-86 88-89 91-92 91-93 95-96 95-97 97-98

g bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 5-8 6-10 8-9 9-10 11-12 11-16 12-13 13-14 14-15
 15-16 19-20 19-23 20-21 21-22 22-23 25-26 25-29 26-27 27-28 28-29 31-32 31-35
 32-33 33-34 34-35 51-52 51-55 52-53 53-54 54-55 58-59 58-62 59-60 60-61 61-62

ct/norm bonds :
 1-2 1-6 2-3 2-68 3-4 3-65 4-5 4-67 5-6 5-8 6-10 8-9 9-10 9-13 11-72 12-71
 14-70 15-73 16-17 17-84 19-20 19-23 20-21 21-22 22-23 25-26 25-29 26-27 27-28
 28-29 31-32 31-35 32-33 33-34 34-35 37-38 37-39 39-40 42-43 42-45 46-47 46-48
 48-49 51-52 51-55 52-53 53-54 53-56 54-55 58-59 58-62 59-60 60-61 60-63 61-62
 74-75 75-76 75-77 79-80 80-81 81-82 85-86 88-89 91-92 91-93 95-96 95-97 97-98

malized bonds :
 11-12 11-16 12-13 13-14 14-15 15-16

lated ring systems :
 containing 1 : 11 : 51 : 58 :

C,N

SH, [*1], [*2], [*3], [*4], [*5], [*6], [*7], [*8], [*9], [*10], [*11], [*12], [*13], [*14]

H, F, CH3, NH2, SH

ch level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
 13:Atom

14:Atom 15:Atom 16:Atom 17:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom
37:CLASS 38:CLASS 39:CLASS 40:CLASS 42:CLASS 43:CLASS 45:CLASS 46:CLASS 47:CLASS
48:CLASS 49:CLASS 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:CLASS 58:Atom 59:Atom
60:Atom 61:Atom 62:Atom 63:CLASS 65:CLASS 67:CLASS 68:CLASS 70:CLASS 71:CLASS
72:CLASS 73:CLASS 74:CLASS 75:CLASS 76:CLASS 77:CLASS 79:CLASS 80:CLASS 81:CLASS
82:CLASS 84:CLASS 85:CLASS 86:CLASS 88:CLASS 89:CLASS 91:CLASS 92:CLASS 93:CLASS
95:CLASS 96:CLASS 97:CLASS 98:CLASS

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 NEWS 2 "Ask CAS" for self-help around the clock
 NEWS 3 JAN 27 Source of Registration (SR) information in REGISTRY updated
 and searchable
 NEWS 4 JAN 27 A new search aid, the Company Name Thesaurus, available in
 CA/CAplus
 NEWS 5 FEB 05 German (DE) application and patent publication number format
 changes
 NEWS 6 MAR 03 MEDLINE and LMedLINE reloaded
 NEWS 7 MAR 03 MEDLINE file segment of TOXCENTER reloaded
 NEWS 8 MAR 03 FRANCEPAT now available on STN
 NEWS 9 MAR 29 Pharmaceutical Substances (PS) now available on STN
 NEWS 10 MAR 29 WPIFV now available on STN
 NEWS 11 MAR 29 New monthly current-awareness alert (SDI) frequency in RAPRA
 NEWS 12 APR 26 PROMT: New display field available
 NEWS 13 APR 26 IFIPAT/IFIUDB/IFICDB: New super search and display field
 available
 NEWS 14 APR 26 LITALERT now available on STN
 NEWS 15 APR 27 NLDB: New search and display fields available
 NEWS 16 May 10 PROUSDDR now available on STN
 NEWS 17 May 10 PROUSDDR: One FREE connect hour, per account, in both May
 and June 2004

NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
 MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
 AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

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STRUCTURE FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9
 DICTIONARY FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
 information enter HELP PROP at an arrow prompt in the file or refer
 to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

=> s l1

SAMPLE SEARCH INITIATED 00:32:07 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 302 TO ITERATE

100.0% PROCESSED 302 ITERATIONS
 SEARCH TIME: 00.00.01

25 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**

PROJECTED ITERATIONS: 4998 TO 7082

PROJECTED ANSWERS: 200 TO 800

L2 25 SEA SSS SAM L1

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 00:32:12 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 6058 TO ITERATE

100.0% PROCESSED 6058 ITERATIONS
 SEARCH TIME: 00.00.01

447 ANSWERS

L3 447 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

168.44	168.65
--------	--------

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

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FILE COVERS 1907 - 12 May 2004 VOL 140 ISS 20
FILE LAST UPDATED: 10 May 2004 (20040510/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4 13 L3

=> s 14 and priestley, e?/au

64 PRIESTLEY, E?/AU

L5 1 L4 AND PRIESTLEY, E?/AU

=> d 15, ibib abs fhitstr, 1

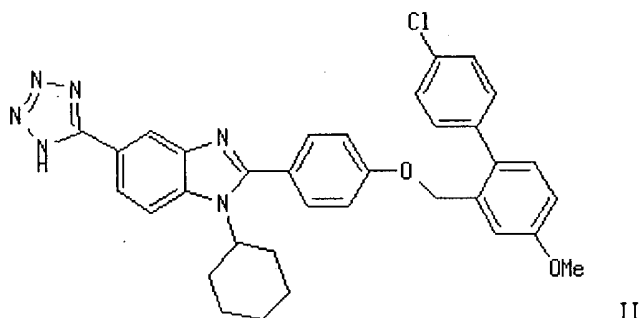
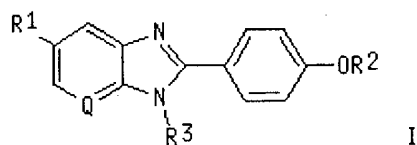
L5 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References

ACCESSION NUMBER: 2003:261620 HCAPLUS
DOCUMENT NUMBER: 138:287673
TITLE: Preparation of phenylbenzimidazole compounds useful for treating hepatitis C virus
INVENTOR(S): Priestley, Eldon Scott; Decicco, Carl P.; Hudyma, Thomas W.; Zheng, Xiaofan
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003026587	A2	20030403	WO 2002-US30989	20020926
WO 2003026587	A3	20031106		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003134853	A1	20030717	US 2002-259041	20020926
US 2004067976	A1	20040408	US 2003-648873	20030827
PRIORITY APPLN. INFO.:		US 2001-324874P P 20010926		
		US 2002-259041 B1 20020926		
OTHER SOURCE(S):		MARPAT 138:287673		

GI



AB Compds. of formula I [Q = CH, N; R1 = tetrazolyl, MeCONHSO2, PhCONHSO2, etc.; R2 = CH2-aryl, CHPh2, etc.; R3 = cycloalkyl] are prepd. which are useful in treating viral hepatitis C. Thus, II was prepd. and had an IC50 of 0.14 μ M against HCV NS5B RdRp (RNA-dependent RNA polymerase).

IT 503857-56-5P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of phenylbenzimidazole compds. for treating hepatitis C viral infection)

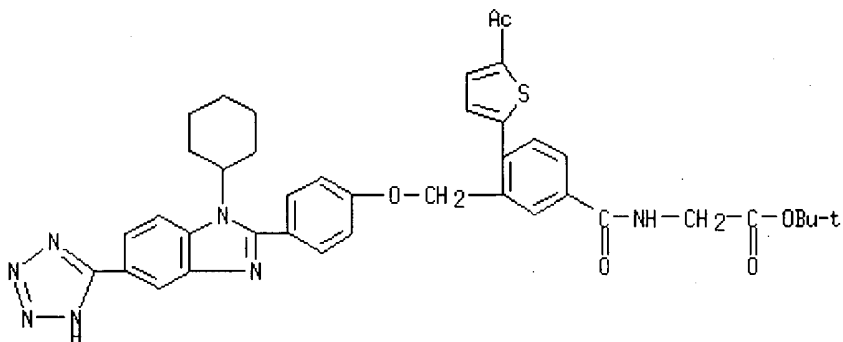
RN 503857-56-5 HCAPLUS

CN Glycine, N-[4-(5-acetyl-2-thienyl)-3-[[4-[1-cyclohexyl-5-(1H-tetrazol-5-yl)-1H-benzimidazol-2-yl]phenoxy]methyl]benzoyl]-, 1,1-dimethylethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 503857-55-4

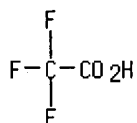
CMF C40 H41 N7 O5 S



CM 2

CRN 76-05-1

CMF C2 H F3 O2



=> d his

(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

L1 STRUCTURE UPLOADED

L2 25 S L1

L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

L4 13 S L3

L5 1 S L4 AND PRIESTLEY, E?/AU

=> s 14 not 15

L6 12 L4 NOT L5

=> s 16 and decicco, c?/au

125 DECICCO, C?/AU

L7 0 L6 AND DECICCO, C?/AU

=> s 16 and hudyma, t?/au

45 HUDYMA, T?/AU

L8 0 L6 AND HUDYMA, T?/AU

=> s 16 and zheng, x?/au

3518 ZHENG, X?/AU

L9 0 L6 AND ZHENG, X?/AU

=> d 16, ibib abs fhitstr, 1-12

L6 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text **Citing References**

ACCESSION NUMBER: 2003:981461 HCAPLUS

DOCUMENT NUMBER: 140:246106

TITLE: Non-nucleoside inhibitors of the hepatitis C virus NS5B polymerase: discovery and preliminary SAR of benzimidazole derivatives

AUTHOR(S): Beaulieu, Pierre L.; Bos, Michael; Bousquet, Yves; Fazal, Gulrez; Gauthier, Jean; Gillard, James; Goulet, Sylvie; LaPlante, Steven; Poupart, Marc-Andre; Lefebvre, Sylvain; McKercher, Ginette; Pellerin, Charles; Austel, Volkhard; Kukolj, George

CORPORATE SOURCE: Department of Chemistry, Research and Development, Boehringer Ingelheim (Canada) Ltd., Laval, QC, H7S 2G5, Can.

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(1), 119-124

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Benzimidazole 5-carboxamide derivs. from a combinatorial screening library were discovered as specific inhibitors of the NS5B polymerase of the hepatitis C virus (HCV). Initial hit-to-lead activities taking advantage of high-throughput parallel synthetic techniques, identified a 1,2-disubstituted benzimidazole 5-carboxylic acid scaffold as the min. core for biol. activity. Potent analogs in this series inhibit the polymerase at low micromolar concns. and provide an attractive 'drug-like' lead structure for further optimization and the development of potential HCV therapeutics.

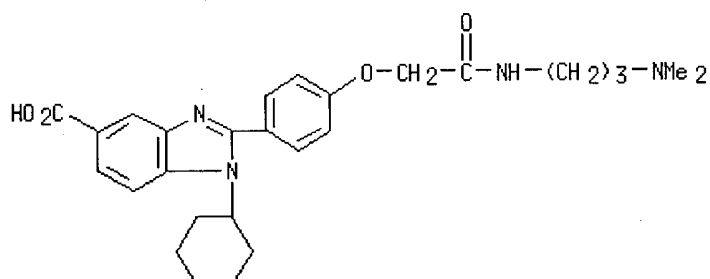
IT **390815-16-4P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(discovery and preliminary SAR of benzimidazole derivs. as inhibitors of hepatitis C virus NS5B polymerase)

RN **390815-16-4 HCAPLUS**

CN 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[4-[2-[[3-(dimethylamino)propyl]amino]-2-oxoethoxy]phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2003:319709 HCAPLUS
DOCUMENT NUMBER: 138:338144
TITLE: Preparation of 2-phenyl benzimidazoles and imidazo-[4,5]pyridines as Cds1/Chk2-inhibitors and adjuvants to chemotherapy or radiation therapy in the treatment of cancer
INVENTOR(S): Arienti, Kristen L.; Axe, Frank U.; Breitenbucher, J. Guy; Huang, Liming; Lee, Alice; McClure, Kelly J.
PATENT ASSIGNEE(S): Ortho-McNeil Pharmaceutical, Inc., USA
SOURCE: PCT Int. Appl., 144 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003032984	A1	20030424	WO 2002-US33371	20021018
WO 2003032984	C1	20031120		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,

PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
 UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
 TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
 CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
 PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
 NE, SN, TD, TG

US 2003176438 A1 20030918 US 2002-273487 20021018

NO 2003002759 A 20030818 NO 2003-2759 20030617

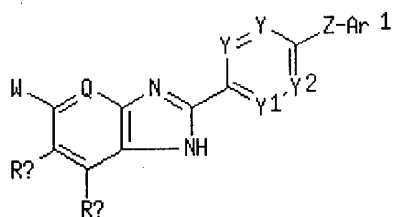
PRIORITY APPLN. INFO.:

US 2001-330304P P 20011019

WO 2002-US33371 W 20021018

OTHER SOURCE(S): MARPAT 138:338144

GI



I

AB 2-Aryl-substituted benzimidazoles and imidazo[4,5]pyridines (shown as I; e.g. 2-[4-(4-chlorophenoxy)phenyl]-1H-benzimidazole-5-carboxylic acid amide (II)) are disclosed as inhibitors of Cds1 and useful as adjuvants to chemotherapy or radiation therapy in the treatment of cancer. For I: W is COOH, -C(O)NHR1, or -SO2NHR1 (R1 is H or C1-4alkyl); Q is N or CH; Ra and Rb are H or halogen; Y, Y1 and Y2 = N and C-Rc with the proviso that 0, 1 or 2 of Y, Y1 and Y2 are N and at least 2 of Rc must be H; Rc = -H, -OH, -C1-6alkyl, -SCF3, halo, -CF3 and -OCF3; Z = O, S, SO, SO2, SO2NR2, NR2SO2, NH, CONR2, piperazinediyl or a covalent bond; R2 is H or C1-4alkyl; Ar1 is an arom. group as defined in the claims. IC50 values are reported for inhibition of human Cds1 checkpoint kinase by 103 examples of I, e.g. 3 nM for 2-[4-(4-chloro-3-trifluoromethylphenoxy)phenyl]-1H-benzimidazole-5-carboxylic acid amide. Addnl. studies were (i) detn. of the effect of II on tumor cell line clonogenic survival, (ii) effect of II on tumor growth in murine xenograft models, (iii) detn. of the effect of 14 examples of I on radiation-induced apoptosis in isolated primary cells, and (iv) detn. of the effect of II on radiation-induced apoptosis in splenocytes in vivo. Although the methods of prepn. are not claimed, ~100 example prepn. are included.

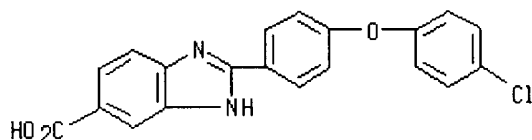
IT **516480-80-1P**, 2-[4-(4-Chlorophenoxy)phenyl]-1H-benzimidazole-5-carboxylic acid

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; prepn. of benzimidazoles and imidazopyridines as Cds1/Chk2-inhibitors and adjuvants to chemotherapy or radiation therapy in treatment of cancer)

RN **516480-80-1** HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(4-chlorophenoxy)phenyl]- (9CI)
 (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing
References

ACCESSION NUMBER: 2003:203407 HCAPLUS
DOCUMENT NUMBER: 138:238181
TITLE: Preparation of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C
INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito
PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
SOURCE: U.S. Pat. Appl. Publ., 406 pp., Cont.-in-part of Appl. No. PCT/JP00/09181.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003050320	A1	20030313	US 2001-939374	20010824
WO 2001047883	A1	20010705	WO 2000-JP9181	20001222
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
JP 2001247550	A2	20010911	JP 2000-391904	20001225
PRIORITY APPLN. INFO.:				
			JP 1999-369008	A 19991227
			WO 2000-JP9181	A2 20001222
			JP 2000-391904	A 20001225
			JP 2001-193786	A 20010626
OTHER SOURCE(S): MARPAT 138:238181				
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, S, CR7, etc.; R1-R4 = H, NO2, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = Ph, cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, CN, etc.; R7 = H, alkyl] are prepd. and formulated. Compds. I showed HCV polymerase inhibitory activity (data

given). E.g., a multi-step synthesis of II.HCl, starting from 2-bromo-5-nitrotoluene and Me 2-(2-fluoro-4-hydroxyphenyl)-1-cyclohexylbenzimidazole-5-carboxylate, was given.

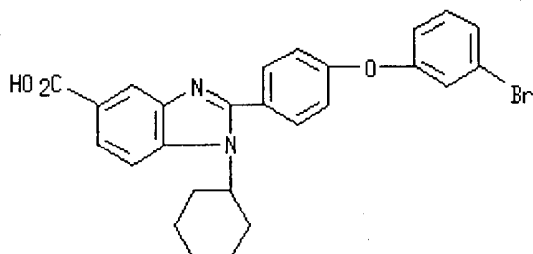
IT 347165-35-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C)

RN 347165-35-9 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(3-bromophenoxy)phenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)



L6 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

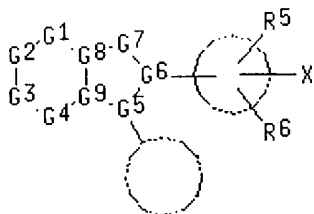
ACCESSION NUMBER: 2003:5773 HCAPLUS
DOCUMENT NUMBER: 138:66657
TITLE: Fused cyclic compounds and medicinal use thereof
INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito
PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
SOURCE: PCT Int. Appl., 603 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003000254	A1	20030103	WO 2002-JP6405	20020626
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2003212846	A2	20030730	JP 2002-185241	20020625
BR 2002005684	A	20030617	BR 2002-5684	20020626
EP 1400241	A1	20040324	EP 2002-743728	20020626
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2004082635	A1	20040429	US 2003-344997	20030218
NO 2003000832	A	20030422	NO 2003-832	20030221

PRIORITY APPLN. INFO.:

JP 2001-193786 A 20010626
 JP 2001-351537 A 20011116
 WO 2002-JP6405 W 20020626

OTHER SOURCE(S): MARPAT 138:66657
 GI



I

AB Fused cyclic compds. represented by the following general formula [I] or pharmaceutically acceptable salts thereof and remedies for hepatitis C contg. these compds.: I wherein each symbol is as defined in the description. Because of having an effect against hepatitis C virus (HVC) based on an HCV polymerase inhibitory effect, these compds. are useful as remedies or preventives for hepatitis C.

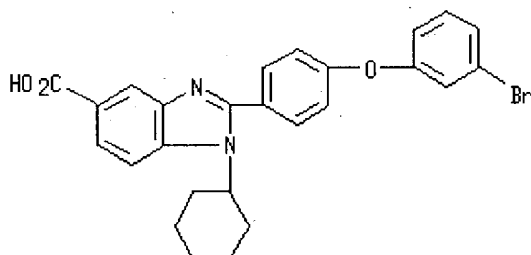
IT 347165-35-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(fused cyclic compds. as hepatitis C virus polymerase inhibitors and antiviral agents)

RN 347165-35-9 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(3-bromophenoxy)phenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

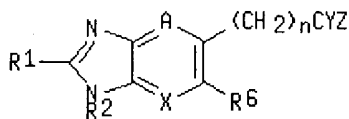
Full Text Citing References

ACCESSION NUMBER: 2002:51438 HCAPLUS
 DOCUMENT NUMBER: 136:118447
 TITLE: Preparation of benzimidazolecarboxylates and related compounds as viral polymerase inhibitors
 INVENTOR(S): Beaulieu, Pierre Louis; Fazal, Gulrez; Gillard, James; Kukolj, George; Austel, Volkhard
 PATENT ASSIGNEE(S): Boehringer Ingelheim (Canada) Ltd., Can.
 SOURCE: PCT Int. Appl., 322 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent

LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004425	A2	20020117	WO 2001-CA989	20010704
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002065418	A1	20020530	US 2001-898297	20010703
US 6448281	B2	20020910		
EP 1301487	A2	20030416	EP 2001-951274	20010704
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004502761	T2	20040129	JP 2002-509292	20010704
US 6479508	B1	20021112	US 2001-995099	20011127
WO 2002070739	A2	20020912	WO 2002-CA323	20020306
WO 2002070739	A3	20030530		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1370682	A2	20031217	EP 2002-712681	20020306
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2003232816	A1	20031218	US 2002-238282	20020910
PRIORITY APPLN. INFO.:				
			US 2000-216084P	P 20000706
			US 2001-274374P	P 20010308
			US 2001-281343P	P 20010405
			US 2001-898297	A3 20010703
			WO 2001-CA989	W 20010704
			US 2001-995099	A3 20011127
			WO 2002-CA323	W 20020306

OTHER SOURCE(S): MARPAT 136:118447
 GI



AB Title compds. [I; X = CH, N; Y = O, S; Z = OH, NH₂, NMe₃, NHR₃, OR₃, 5-6 membered (substituted) heterocyclyl; A = N, COR₇, CR₅; R₅ = H, halo, alkyl; R₇ = H, alkyl; X and A are not both N; R₆ = H, halo, alkyl, OR₇; R₇ = H, alkyl; R₁ = (substituted) hetero(bi)cyclyl, Ph, phenylalkyl, alkenyl, phenylalkenyl, cycloalkyl, alkyl, CF₃; R₂ = (substituted) alkyl,

cycloalkyl, cycloalkylalkyl, bicycloalkyl, adamantyl, Ph, pyridyl; R3 = H, alkyl, cycloalkyl, cycloalkylalkyl, aryl, arylalkyl, alkenyl, cycloalkylalkenyl, arylalkenyl, dialkylamino, heterocyclyl, etc.; n = 0, 1], were prepd. Thus, Me 3-amino-4-cyclohexylaminobenzoate (prepn. given), 2-pyridinecarboxaldehyde, and Oxone were stirred in DMF to give 80% Et 1-cyclohexyl-2-pyridin-2-yl-1H-benzimidazole-5-carboxylate, which was sapond. with aq. NaOH in MeOH to give 91% 1-cyclohexyl-2-pyridin-2-yl-1H-benzimidazole-5-carboxylic acid. The latter inhibited hepatitis C virus RNA dependent polymerase (NS5B) with IC50 = 1-5 μ M.

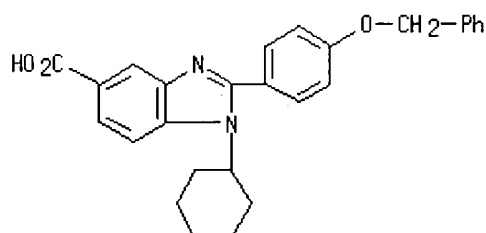
IT 347166-09-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzimidazolecarboxylates and related compds. as viral polymerase inhibitors)

RN 347166-09-0 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2001:489367 HCAPLUS
 DOCUMENT NUMBER: 135:76874
 TITLE: Preparation of heterocyclic compounds as remedies for hepatitis C
 INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito
 PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
 SOURCE: PCT Int. Appl., 438 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001047883	A1	20010705	WO 2000-JP9181	20001222
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1162196	A1	20011212	EP 2000-987728	20001222

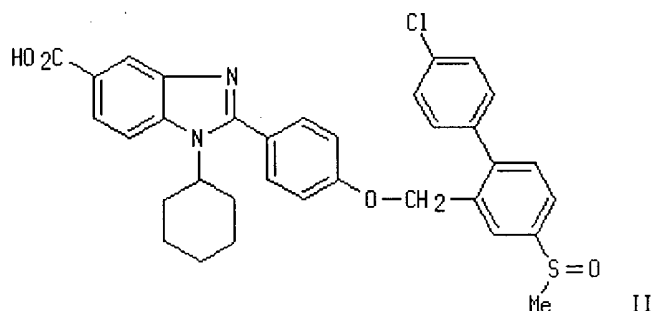
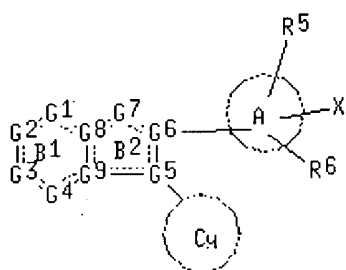
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO

<u>BR 2000008525</u>	A	20020102	<u>BR 2000-8525</u>	20001222
<u>TR 200103147</u>	T1	20020621	<u>TR 2001-200103147</u>	20001222
<u>NZ 514403</u>	A	20021025	<u>NZ 2000-514403</u>	20001222
<u>AU 763356</u>	B2	20030717	<u>AU 2001-24017</u>	20001222
<u>RU 2223761</u>	C2	20040220	<u>RU 2001-126283</u>	20001222
<u>NO 2001004134</u>	A	20011022	<u>NO 2001-4134</u>	20010824
<u>US 2003050320</u>	A1	20030313	<u>US 2001-939374</u>	20010824
<u>ZA 2001007870</u>	A	20020925	<u>ZA 2001-7870</u>	20010928

PRIORITY APPLN. INFO.:

<u>JP 1999-369008</u>	A	19991227
<u>WO 2000-JP9181</u>	W	20001222
<u>JP 2000-391904</u>	A	20001225
<u>JP 2001-193786</u>	A	20010626

OTHER SOURCE(S) : MARPAT 135:76874
GI



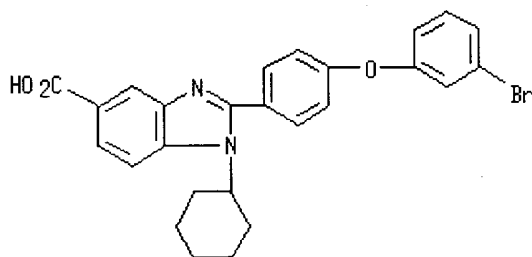
AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, etc.; R1 - R4 = H, nitro, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = C3-C8 cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, cyano, etc.] are prepd. The benzimidazole deriv. II in vitro showed IC50 of 0.011 μ M against hepatitis C virus polymerase. A formulation is given.

IT 347165-35-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of heterocyclic compds. as remedies for hepatitis C)

RN 347165-35-9 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(3-bromophenoxy)phenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

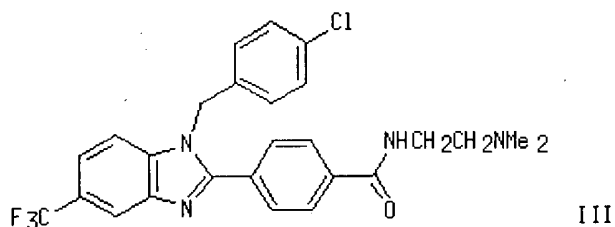
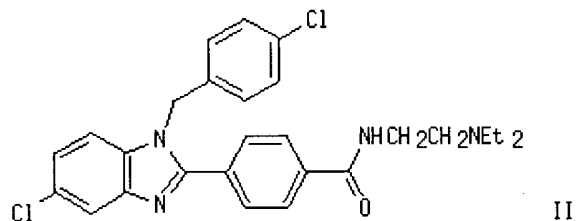
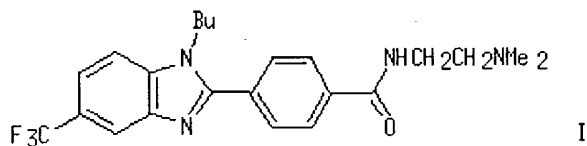
27

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2001:412102 HCAPLUS
DOCUMENT NUMBER: 135:177890
TITLE: Synthesis and antimicrobial activity of some new
2-phenyl-N-substituted carboxamido-1H-benzimidazole
derivatives
AUTHOR(S): Goker, Hakan; Tunchilek, Meral; Suzen, Sibel; Kus,
Canan; Altanlar, Nurten
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of
Pharmacy, Ankara University, Ankara, 06100, Turk.
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (2001),
334(5), 148-152
CODEN: ARPMAS; ISSN: 0365-6233
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:177890
GI



AB Some 1H-benzimidazole-carboxamide derivs. were prepd. and their
antimicrobial activities against Staphylococcus aureus, Escherichia coli,

and *Candida albicans* evaluated. Compds. I, II, and III exhibited the best activity against *C. albicans*.

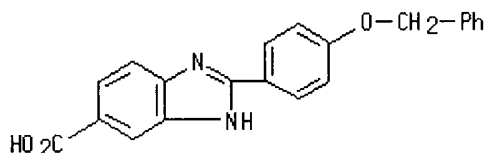
IT 174422-18-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and antimicrobial activity of new 2-phenyl-N-substituted carboxamido-1H-benzimidazole derivs.)

RN 174422-18-5 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]- (9CI)
(CA INDEX NAME)

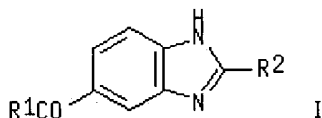


REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing
References

ACCESSION NUMBER: 1999:614608 HCAPLUS
DOCUMENT NUMBER: 131:286454
TITLE: Synthesis and antimicrobial activity of some new benzimidazole carboxylates and carboxamides
AUTHOR(S): Ayhan-Kilcigil, Gulgun; Tuncbilek, Meral; Altanlar, Nurten; Goker, Hakan
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Ankara University, Ankara, 06100, Turk.
SOURCE: Farmaco (1999), 54(8), 562-565
CODEN: FRMCE8; ISSN: 0014-827X
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Benzimidazole carboxylates and carboxamides, e.g., I [R1 = MeO, (2-pyridinylmethyl)amino, 4-methylpiperidino, R2 = 2-ClC6H4, 4-ClC6H4, 2,4-Cl2C6H3, 2-MeOC6H4, 4-MeOC6H4, 2-thienyl], were synthesized and evaluated for their antimicrobial activities against *Staphylococcus aureus*, *Escherichia coli*, and *Candida albicans*. Among the investigated compds., I (R1 = MeO, R2 = 2-MeOC6H4) exhibited best activity against *C. albicans*.

IT 246517-85-1P

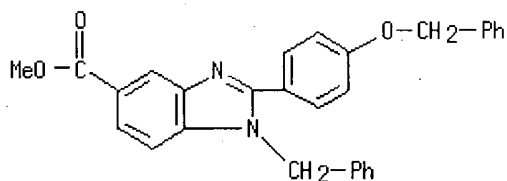
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and antimicrobial activity of benzimidazole carboxylates and carboxamides)

RN 246517-85-1 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]-1-

(phenylmethyl)-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

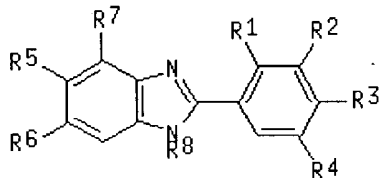
L6 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 1999:184240 HCAPLUS
 DOCUMENT NUMBER: 130:209707
 TITLE: Preparation of 2-substituted phenyl-benzimidazole antibacterial agents
 INVENTOR(S): Ohemeng, Kwasi Adomako; Nguyen, Van Nhatton
 PATENT ASSIGNEE(S): Ortho-McNeil Pharmaceutical, Inc., USA
 SOURCE: PCT Int. Appl., 70 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9911627	A1	19990311	WO 1998-US18586	19980904
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, GM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 5942532	A	19990824	US 1997-924558	19970905
AU 9893054	A1	19990322	AU 1998-93054	19980904
PRIORITY APPLN. INFO.:			US 1997-924558	19970905
			WO 1998-US18586	19980904

OTHER SOURCE(S): MARPAT 130:209707
 GI



Chak

AB Benzimidazoles I [R1 = H, OH, alkoxy; R2, R3, R4 = H, OH, alkyl, CF3, halo, etc.; R5 = H, amino, amidino; R6 = nitro, C(NHR9):NR10; R7 = H, amino, nitro; R8 = H, Me], antibacterial compds., were prepd. These compds. are effective in inhibiting the action of a bacterial histidine protein kinase and are useful as anti-infective agents against a variety

of bacterial organisms, including organisms which are resistant to other known antibiotics. E.g., 3,4-diaminobenzimidate, prepd. from 3,4-diaminobenzonitrile, was treated with NH_3/EtOH , then with 4-Me $_3\text{CC}_6\text{H}_4\text{CHO}$ to give 2-[4-(1,1-dimethylethyl)phenyl]-2H-benzimidazole-5-carboximidamide.

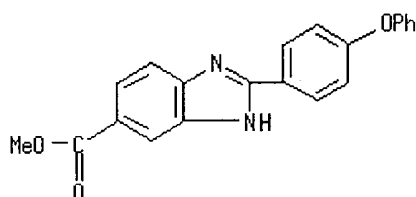
IT 220955-73-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of phenylbenzimidazoles as antibacterial agents)

RN 220955-73-7 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-(4-phenoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)



103(a) Bioisoster

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 1998:634393 HCAPLUS
 DOCUMENT NUMBER: 129:316174
 TITLE: Synthesis of some new benzimidazolecarboxamides and evaluation of their antimicrobial activity
 AUTHOR(S): Goker, Hakan; Tunchilek, Meral; Ayhan, Gulgun; Altanlar, Nurten
 CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Ankara University, Ankara, 06100, Turk.
 SOURCE: Farmaco (1998), 53(6), 415-420
 CODEN: FRMCE8; ISSN: 0014-827X
 PUBLISHER: Elsevier Science S.A.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

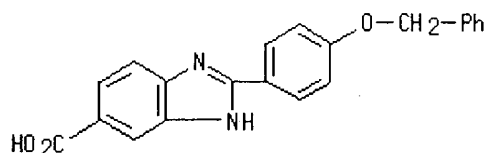
AB A series of 1,2-disubstituted benzimidazole-5(6)-carboxamides was prepd. and evaluated in vitro for antimicrobial activity against Staphylococcus aureus, Escherichia coli, and Candida albicans. The precursor benzimidazolecarboxylic acids were prepd. via oxidative condensation of diaminobenzoic acids with aldehydes and via several steps over the 2(1H)-benzimidazolones, resp. All acids were converted to their acyl chlorides with SOCl_2 , then amidified with several N,N'-dialkylaminoethyl derivs.

IT 174422-18-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. and bactericidal and fungicidal activity of benzimidazolecarboxamides)

RN 174422-18-5 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 1996:144268 HCAPLUS
 DOCUMENT NUMBER: 124:197998
 TITLE: Synthesis of 1,2-disubstituted benzimidazole-5(6)-carboxamides and evaluation of their antimicrobial activity
 AUTHOR(S): Goeker, Hakan; Tebrizli, Emin; Abbasoglu, Ufuk
 CORPORATE SOURCE: Faculty of Pharmacy, Univ. of Ankara, Tandogan, 06100, Turk.
 SOURCE: Farmaco (1996), 51(1), 53-8
 CODEN: FRMCE8
 PUBLISHER: Societa Chimica Italiana
 DOCUMENT TYPE: Journal
 LANGUAGE: English

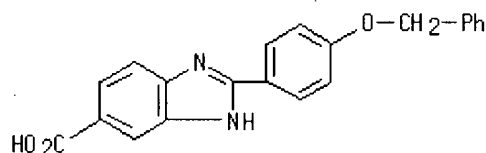
AB Fourteen N'-(N,N-dialkylaminoethyl)-benzimidazole 5(6)- or 5-carboxamides having several substituents on the azole and benzene nuclei were prepd. and evaluated in vitro for antimicrobial activity. The precursor benzimidazolecarboxylic acids were prepd. via oxidative condensation of diaminobenzoic acids and several aldehydes with cupric ion. All carboxamides were prepd. from the corresponding acids and N,N-dialkylethylenediamine. Antibacterial and antifungal activities were detd. as MIC values. Comps. which were prepd. by replacement with bulky alkyl groups on the tert-N benzimidazole atom gave the best results.

IT 174422-18-5P

RL: PRP (Properties); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (synthesis of 1,2-disubstituted benzimidazole-5(6)-carboxamides and evaluation of their antimicrobial activity)

RN 174422-18-5 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]- (9CI)
 (CA INDEX NAME)

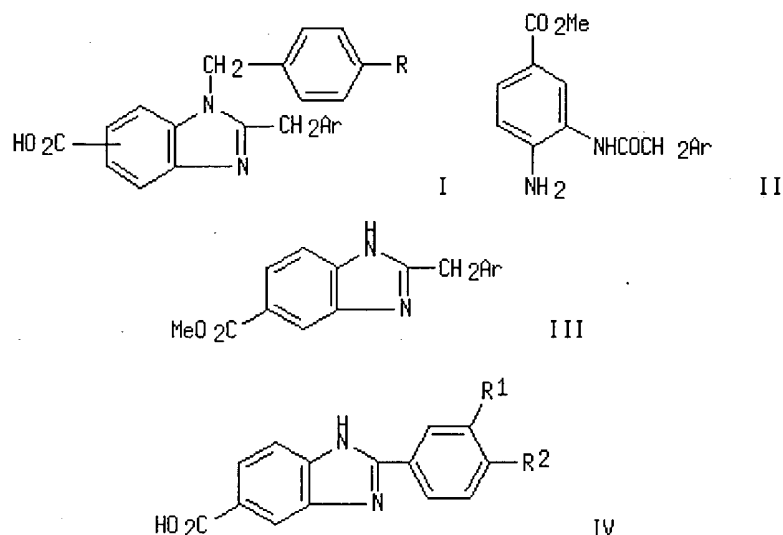


L6 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 1996:38013 HCAPLUS
 DOCUMENT NUMBER: 124:202112
 TITLE: Synthesis of some new benzimidazole-5(6)-carboxylic acids
 AUTHOR(S): Goeker, Hakan; Oelgen, Suereyya; Ertan, Rahmiye; Akguen, Huelya; Oezbey, Sueheyla; Kendi, Engin; Topcu, Guel

CORPORATE SOURCE: Fac. Pharmacy, Ankara Univ., Ankara, 06100, Turk.
 SOURCE: Journal of Heterocyclic Chemistry (1995), 32(6),
 1767-73
 CODEN: JHTCAD; ISSN: 0022-152X
 PUBLISHER: HeteroCorporation
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



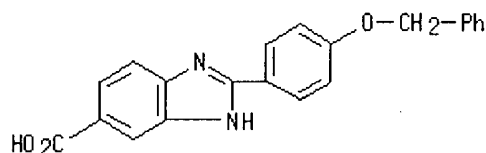
AB The title compds., 1,2-dialkyl-benzimidazole-5(6)-carboxylic acids I (Ar = Ph, 4-MeC₆H₄, 4-ClC₆H₄, 2-BrC₆H₄, OPh, 4-ClC₆H₄O, etc., R = H, F, CO₂H position = 5, 6) were prepd. in four steps; (1) prepn. of mono amide derivs. II by the reaction of Me 3,4-diaminobenzoate and substituted Ph or phenoxyacetic acid chlorides ArCH₂COCl, (2) prepn. of the Me benzimidazolecarboxylates III, with zinc chloride and dry hydrogen chloride gas, (3) alk. hydrolysis of the esters, and (4) substitution of the imidazole ring with benzyl or p-fluorobenzyl bromide, in alkali medium. 2-Aryl-benzimidazole-5(6)-carboxylic acids IV (R₁ = H, OCH₂Ph, OH, R₂ = OCH₂Ph, OH) were prepd. via the oxidative condensation of 3,4-diaminobenzoic acid and arom. aldehydes with cupric ion.

IT 174422-18-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of benzimidazolecarboxylic acids)

RN 174422-18-5 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]- (9CI)
 (CA INDEX NAME)



=> file caold

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	ENTRY	SESSION
FULL ESTIMATED COST	68.91	237.56
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-9.01	-9.01

FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004
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FILE COVERS 1907-1966
 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

L1 STRUCTURE UPLOADED
 L2 25 S L1
 L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

L4 13 S L3
 L5 1 S L4 AND PRIESTLEY, E?/AU
 L6 12 S L4 NOT L5
 L7 0 S L6 AND DECICCO, C?/AU
 L8 0 S L6 AND HUDYMA, T?/AU
 L9 0 S L6 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004

=> s l3

L10 0 L3

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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9
DICTIONARY FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

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L11 HAS NO ANSWERS

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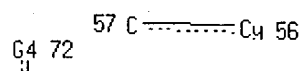
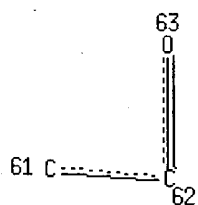
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55 G2

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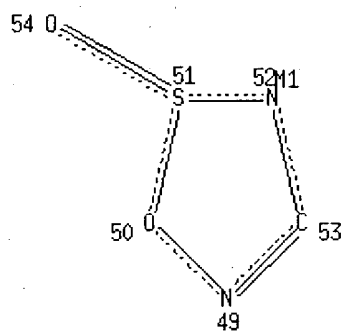


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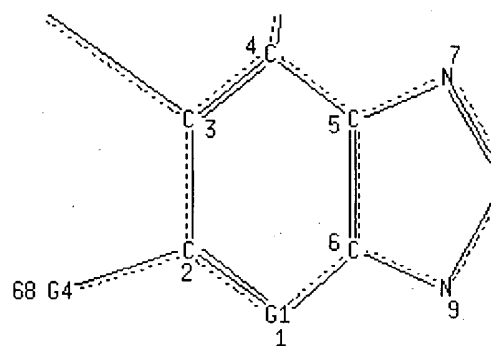
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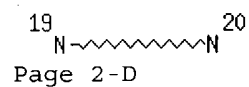
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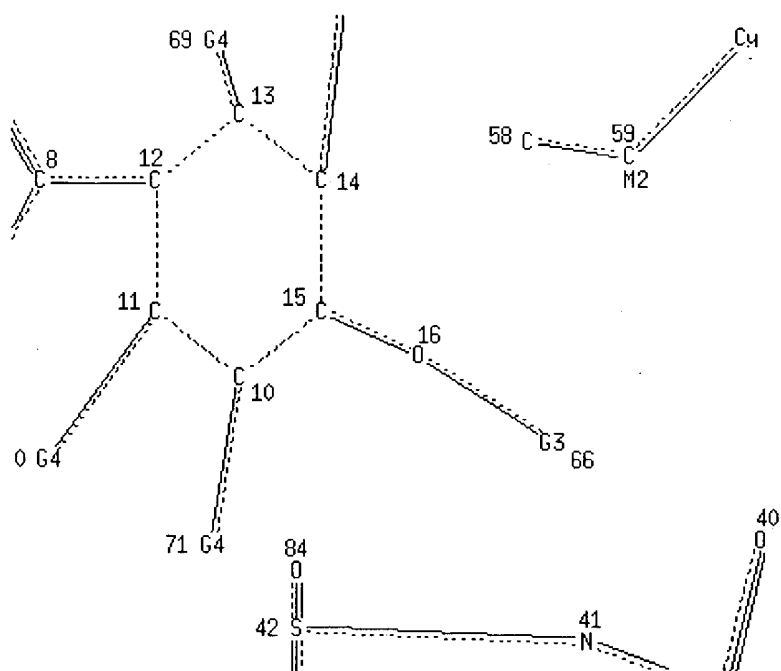
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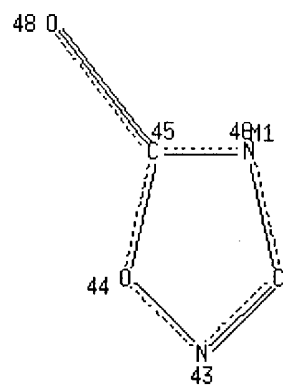
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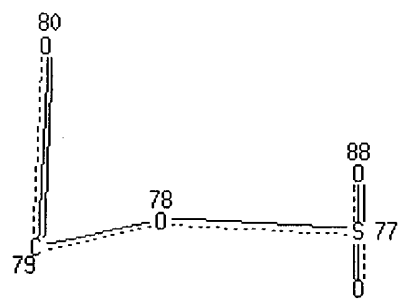
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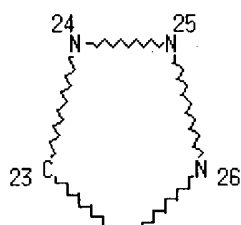
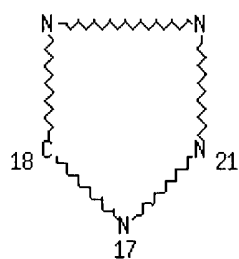
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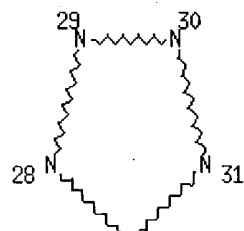
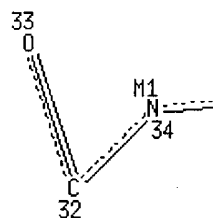
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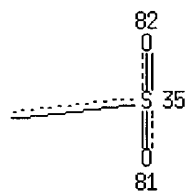
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Page 3-D

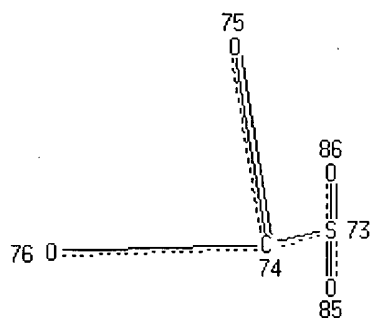


Page 3-E



Page 3-F

87



Page 4-B



Page 4-D



Page 4-E

VAR G1=89/90

VAR G2=18/24/29/35/36/42/47/53/73/77

VAR G3=91/57/58/61/64

VAR G4=92/93/94/95

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NUMBER OF NODES IS  95

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STEREO ATTRIBUTES: NONE

=> s l11

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SAMPLE SCREEN SEARCH COMPLETED -    302 TO ITERATE

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100.0% PROCESSED      302 ITERATIONS                      37 ANSWERS
SEARCH TIME: 00.00.01

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FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:   4998 TO    7082
PROJECTED ANSWERS:      376 TO    1104

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L12 37 SEA SSS SAM L11

=> s l11 full

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THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 00:47:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    6058 TO ITERATE

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100.0% PROCESSED      6058 ITERATIONS                      595 ANSWERS
SEARCH TIME: 00.00.01

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L13 595 SEA SSS FUL L11

=> d his

(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

L1 STRUCTURE UPLOADED

L2 25 S L1
L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

L4 13 S L3
L5 1 S L4 AND PRIESTLEY, E?/AU
L6 12 S L4 NOT L5
L7 0 S L6 AND DECICCO, C?/AU
L8 0 S L6 AND HUDYMA, T?/AU
L9 0 S L6 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004

L10 0 S L3

FILE 'REGISTRY' ENTERED AT 00:33:56 ON 12 MAY 2004

L11 STRUCTURE UPLOADED
L12 37 S L11
L13 595 S L11 FULL

=> s l13 not l3
L14 148 L13 NOT L3

=> file hcaplus		
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	ENTRY	SESSION
FULL ESTIMATED COST	164.66	402.64
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-9.01

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FILE COVERS 1907 - 12 May 2004 VOL 140 ISS 20
FILE LAST UPDATED: 10 May 2004 (20040510/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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5 L14
591649 THU/RL
L15 5 L14/THU
(L14 (L) THU/RL)

=> s l15 and priestley, e?/au
 64 PRIESTLEY, E?/AU
 L16 1 L15 AND PRIESTLEY, E?/AU

=> d his

(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

L1 STRUCTURE UPLOADED
 L2 25 S L1
 L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

L4 13 S L3
 L5 1 S L4 AND PRIESTLEY, E?/AU
 L6 12 S L4 NOT L5
 L7 0 S L6 AND DECICCO, C?/AU
 L8 0 S L6 AND HUDYMA, T?/AU
 L9 0 S L6 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004

L10 0 S L3

FILE 'REGISTRY' ENTERED AT 00:33:56 ON 12 MAY 2004

L11 STRUCTURE UPLOADED
 L12 37 S L11
 L13 595 S L11 FULL
 L14 148 S L13 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:47:52 ON 12 MAY 2004

L15 5 S L14/THU
 L16 1 S L15 AND PRIESTLEY, E?/AU

=> s l16 not l5

L17 0 L16 NOT L5

=> d l16, ibib abs fhitstr, 1

L16 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER:	2003:261620 HCAPLUS
DOCUMENT NUMBER:	138:287673
TITLE:	Preparation of phenylbenzimidazole compounds useful for treating hepatitis C virus
INVENTOR(S):	Priestley, Eldon Scott; Decicco, Carl P.; Hudyma, Thomas W.; Zheng, Xiaofan
PATENT ASSIGNEE(S):	Bristol-Myers Squibb Company, USA
SOURCE:	PCT Int. Appl., 74 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003026587	A2	20030403	WO 2002-US30989	20020926
WO 2003026587	A3	20031106		

NO

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US 2003134853 A1 20030717 US 2002-259041 20020926

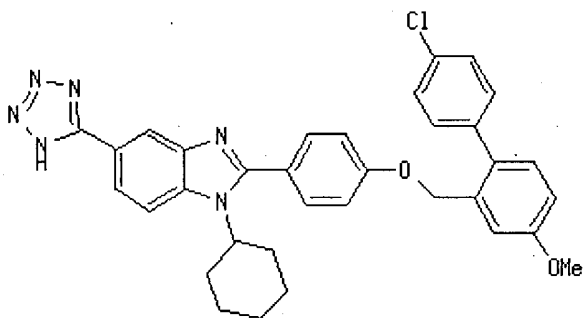
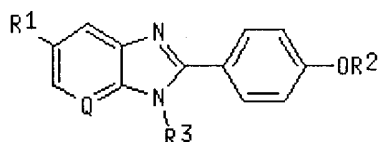
US 2004067976 A1 20040408 US 2003-648873 20030827

PRIORITY APPLN. INFO.: US 2001-324874P P 20010926

US 2002-259041 B1 20020926

OTHER SOURCE(S): MARPAT 138:287673

GI



AB Compds. of formula I [Q = CH, N; R1 = tetrazolyl, MeCONHSO2, PhCONHSO2, etc.; R2 = CH2-aryl, CHPh2, etc.; R3 = cycloalkyl] are prepd. which are useful in treating viral hepatitis C. Thus, II was prepd. and had an IC50 of 0.14 μ M against HCV NS5B RdRp (RNA-dependent RNA polymerase).

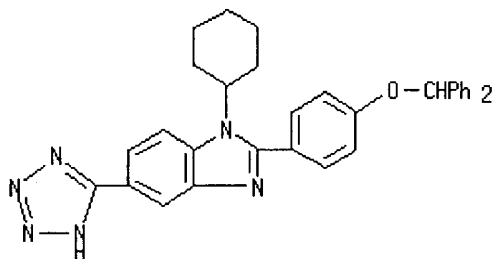
IT **503857-49-6P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); **THU** (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of phenylbenzimidazole compds. for treating hepatitis C viral infection)

RN **503857-49-6** HCAPLUS

CN 1H-Benzimidazole, 1-cyclohexyl-2-[4-(diphenylmethoxy)phenyl]-5-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



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(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

L1 STRUCTURE UPLOADED
L2 25 S L1
L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

L4 13 S L3
L5 1 S L4 AND PRIESTLEY, E?/AU
L6 12 S L4 NOT L5
L7 0 S L6 AND DECICCO, C?/AU
L8 0 S L6 AND HUDYMA, T?/AU
L9 0 S L6 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004

L10 0 S L3

FILE 'REGISTRY' ENTERED AT 00:33:56 ON 12 MAY 2004

L11 STRUCTURE UPLOADED
L12 37 S L11
L13 595 S L11 FULL
L14 148 S L13 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:47:52 ON 12 MAY 2004

L15 5 S L14/THU
L16 1 S L15 AND PRIESTLEY, E?/AU
L17 0 S L16 NOT L5

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L18 4 L15 NOT L16

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125 DECICCO, C?/AU
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L20 0 L19 NOT L16

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0 HYDYMA, T?/AU
L21 0 L18 AND HYDYMA, T?/AU

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3518 ZHENG, X?/AU
L22 0 L18 AND ZHENG, X?/AU

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L18 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2003:970508 HCAPLUS

DOCUMENT NUMBER: 140:174511

TITLE: Mechanism of action and antiviral activity of benzimidazole-based allosteric inhibitors of the hepatitis C virus RNA-dependent RNA polymerase

AUTHOR(S): Tomei, Licia; Altamura, Sergio; Bartholomew, Linda; Biroccio, Antonino; Ceccacci, Alessandra; Pacini, Laura; Narjes, Frank; Gennari, Nadia; Bisbocci, Monica; Incitti, Ilario; Orsatti, Laura; Harper, Steven; Stansfield, Ian; Rowley, Michael; De Francesco, Raffaele; Migliaccio, Giovanni

CORPORATE SOURCE: Istituto di Ricerche di Biologia Molecolare "P. Angeletti", Pomezia-Rome, 00040, Italy

SOURCE: Journal of Virology (2003), 77(24), 13225-13231
CODEN: JOVIAM; ISSN: 0022-538X

PUBLISHER: American Society for Microbiology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The RNA-dependent RNA polymerase of hepatitis C virus (HCV) is the catalytic subunit of the viral RNA amplification machinery and is an appealing target for the development of new therapeutic agents against HCV infection. Nonnucleoside inhibitors based on a benzimidazole scaffold have been recently reported. Compds. of this class are efficient inhibitors of HCV RNA replication in cell culture, thus providing attractive candidates for further development. Here we report the detailed anal. of the mechanism of action of selected benzimidazole inhibitors. Kinetic data and binding expts. indicated that these compds. act as allosteric inhibitors that block the activity of the polymerase prior to the elongation step. Escape mutations that confer resistance to these compds. map to proline 495, a residue located on the surface of the polymerase thumb domain and away from the active site. Substitution of this residue is sufficient to make the HCV enzyme and replicons resistant to the inhibitors. Interestingly, proline 495 lies in a recently identified noncatalytic GTP-binding site, thus validating it as a potential allosteric site that can be targeted by small-mol. inhibitors of HCV polymerase.

IT 658693-60-8

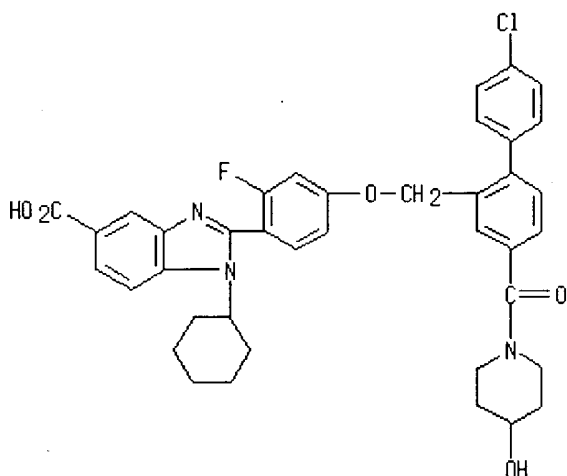
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity);

THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(mechanism of action and antiviral activity of benzimidazole-based allosteric inhibitors of hepatitis C virus RNA-dependent RNA polymerase)

RN 658693-60-8 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-[[4'-chloro-4-[(4-hydroxy-1-piperidinyl)carbonyl][1,1'-biphenyl]-2-yl]methoxy]-2-fluorophenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2003:203407 HCAPLUS
 DOCUMENT NUMBER: 138:238181
 TITLE: Preparation of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C
 INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito
 PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
 SOURCE: U.S. Pat. Appl. Publ., 406 pp., Cont.-in-part of Appl. No. PCT/JP00/09181.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003050320	A1	20030313	US 2001-939374	20010824
WO 2001047883	A1	20010705	WO 2000-JP9181	20001222
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
JP 2001247550	A2	20010911	JP 2000-391904	20001225
PRIORITY APPLN. INFO.:				
			JP 1999-369008	A 19991227
			WO 2000-JP9181	A2 20001222
			JP 2000-391904	A 20001225
			JP 2001-193786	A 20010626

OTHER SOURCE(S): MARPAT 138:238181
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

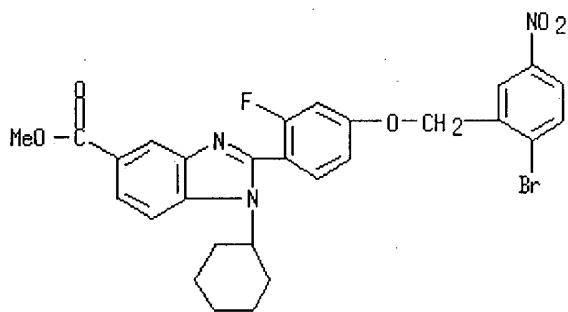
AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, S, CR7, etc.; R1-R4 = H, NO2, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = Ph, cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, CN, etc.; R7 = H, alkyl] are prepd. and formulated. Compds. I showed HCV polymerase inhibitory activity (data given). E.g., a multi-step synthesis of II.HCl, starting from 2-bromo-5-nitrotoluene and Me 2-(2-fluoro-4-hydroxyphenyl)-1-cyclohexylbenzimidazole-5-carboxylate, was given.

IT 480461-26-5P

RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C)

RN 480461-26-5 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-[(2-bromo-5-nitrophenyl)methoxy]-2-fluorophenyl]-1-cyclohexyl-, methyl ester (9CI) (CA INDEX NAME)



Yes Piroisostero

L18 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2003:5773 HCAPLUS
DOCUMENT NUMBER: 138:66657
TITLE: Fused cyclic compounds and medicinal use thereof
INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito
PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
SOURCE: PCT Int. Appl., 603 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003000254	A1	20030103	WO 2002-JP6405	20020626
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG,				

US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
 CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

JP 2003212846	A2	20030730	JP 2002-185241	20020625
BR 2002005684	A	20030617	BR 2002-5684	20020626
EP 1400241	A1	20040324	EP 2002-743728	20020626

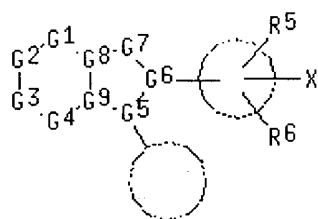
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US 2004082635	A1	20040429	US 2003-344997	20030218
NO 2003000832	A	20030422	NO 2003-832	20030221

PRIORITY APPLN. INFO.:

JP 2001-193786	A	20010626
JP 2001-351537	A	20011116
WO 2002-JP6405	W	20020626

OTHER SOURCE(S): MARPAT 138:66657
 GI



I

AB Fused cyclic compds. represented by the following general formula [I] or pharmaceutically acceptable salts thereof and remedies for hepatitis C contg. these compds.: I wherein each symbol is as defined in the description. Because of having an effect against hepatitis C virus (HVC) based on an HCV polymerase inhibitory effect, these compds. are useful as remedies or preventives for hepatitis C.

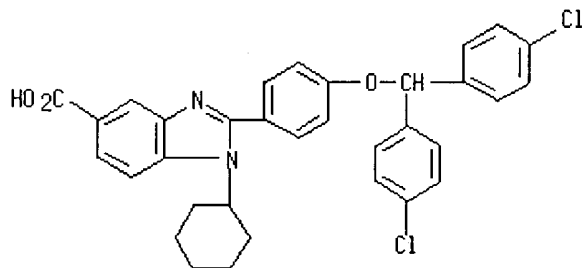
IT 347166-38-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(fused cyclic compds. as hepatitis C virus polymerase inhibitors and antiviral agents)

RN 347166-38-5 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-[bis(4-chlorophenyl)methoxy]phenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)



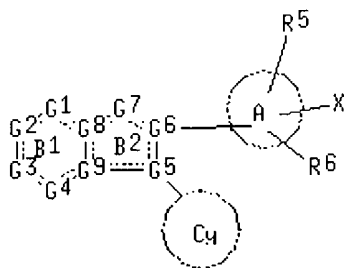
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L18 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

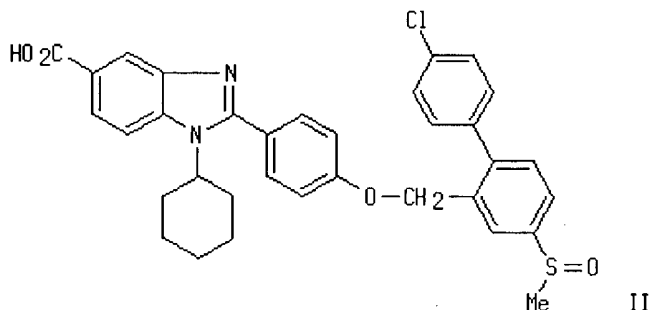
Full Text	Citing References
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ACCESSION NUMBER: 2001:489367 HCAPLUS
 DOCUMENT NUMBER: 135:76874
 TITLE: Preparation of heterocyclic compounds as remedies for hepatitis C
 INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito
 PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
 SOURCE: PCT Int. Appl., 438 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 2001047883</u>	A1	20010705	<u>WO 2000-JP9181</u>	20001222
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<u>EP 1162196</u>	A1	20011212	<u>EP 2000-987728</u>	20001222
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<u>TR 200103147</u>	T1	20020621	<u>TR 2001-200103147</u>	20001222
<u>NZ 514403</u>	A	20021025	<u>NZ 2000-514403</u>	20001222
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<u>NO 2001004134</u>	A	20011022	<u>NO 2001-4134</u>	20010824
<u>US 2003050320</u>	A1	20030313	<u>US 2001-939374</u>	20010824
<u>ZA 2001007870</u>	A	20020925	<u>ZA 2001-7870</u>	20010928
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			<u>WO 2000-JP9181</u>	W 20001222
			<u>JP 2000-391904</u>	A 20001225
			<u>JP 2001-193786</u>	A 20010626
OTHER SOURCE(S):		MARPAT 135:76874		
GI				



I



II

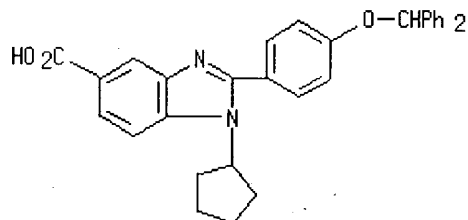
AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, etc.; R1 - R4 = H, nitro, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = C3-C8 cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, cyano, etc.] are prepd. The benzimidazole deriv. II in vitro showed IC50 of 0.011 μ M against hepatitis C virus polymerase. A formulation is given.

IT **347165-90-6P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of heterocyclic compds. as remedies for hepatitis C)

RN **347165-90-6** HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 1-cyclopentyl-2-[4-(diphenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

27

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS

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FULL ESTIMATED COST

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SESSION

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FILE COVERS 1907-1966
 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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 L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

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 L5 1 S L4 AND PRIESTLEY, E?/AU
 L6 12 S L4 NOT L5
 L7 0 S L6 AND DECICCO, C?/AU
 L8 0 S L6 AND HUDYMA, T?/AU
 L9 0 S L6 AND ZHENG, X?/AU

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FILE 'REGISTRY' ENTERED AT 00:33:56 ON 12 MAY 2004

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 L13 595 S L11 FULL
 L14 148 S L13 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:47:52 ON 12 MAY 2004

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 L17 0 S L16 NOT L5
 L18 4 S L15 NOT L16
 L19 1 S L15 AND DECICCO, C?/AU
 L20 0 S L19 NOT L16
 L21 0 S L18 AND HYDYMA, T?/AU
 L22 0 S L18 AND ZHENG, X?/AU

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STRUCTURE FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9

DICTIONARY FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Crossover limits have been increased. See [HELP CROSSOVER](#) for details.

Experimental and calculated property data are now available. For more information enter [HELP PROP](#) at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

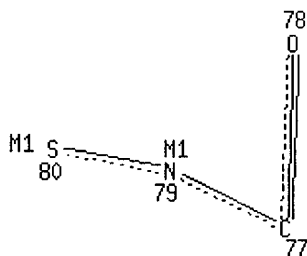
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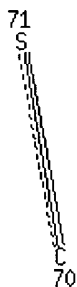


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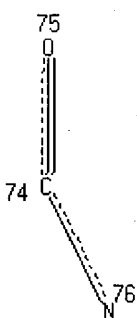
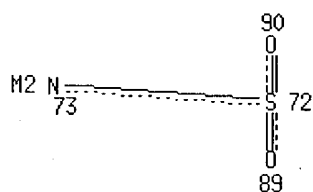
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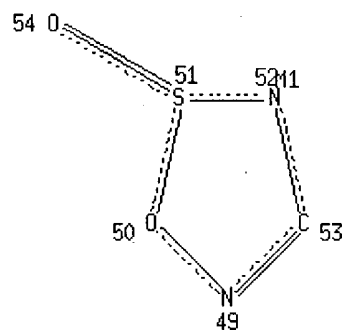
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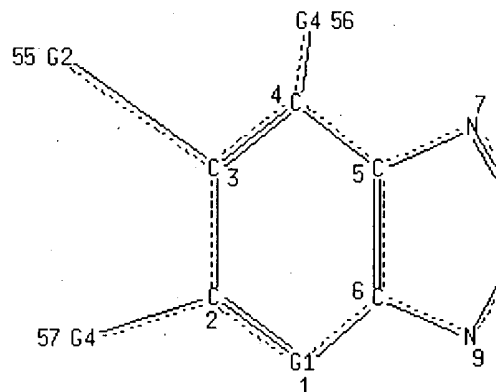
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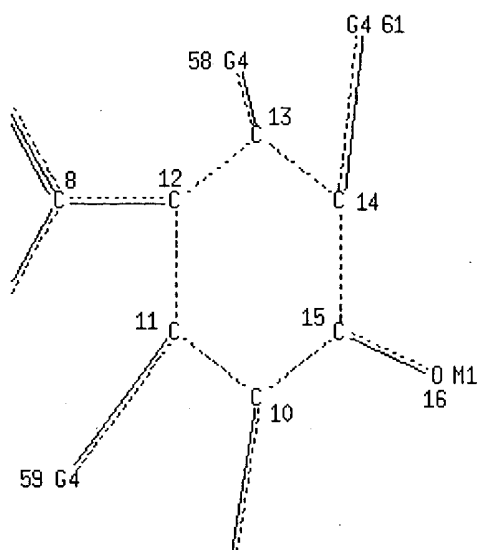


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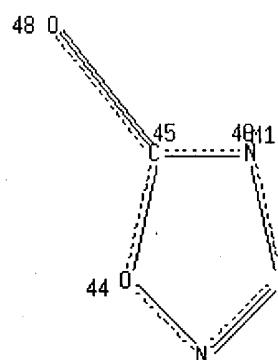
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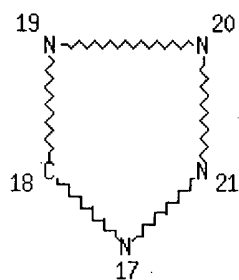


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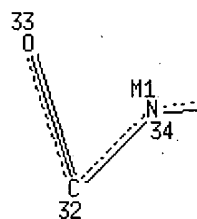
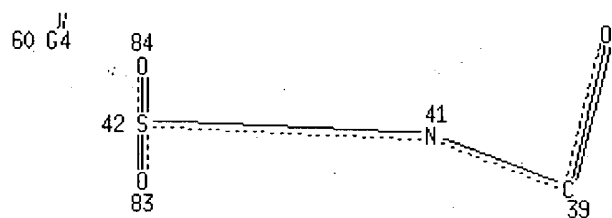
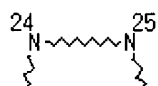


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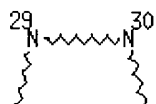
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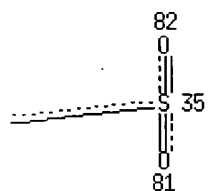
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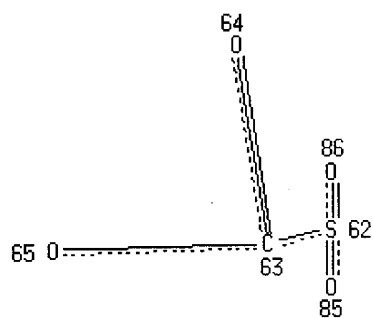
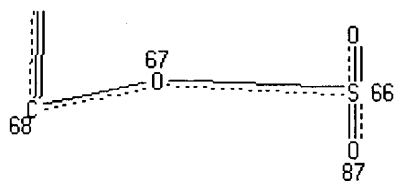
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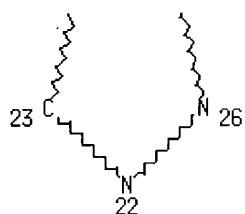
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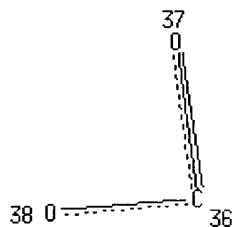
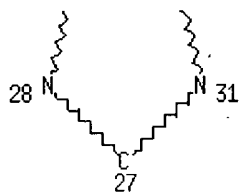
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Page 4-D



Page 4-E

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NSPEC	IS C	AT	70
NSPEC	IS C	AT	71
NSPEC	IS C	AT	72
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 MLEVEL IS CLASS AT 16 32 33 34 35 36 37 38 39 40 41 42 48 54 62 63 64
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 86 87 88 89 90 93 94 95 96 97 98
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 10 8 43 49
 NUMBER OF NODES IS 98

STEREO ATTRIBUTES: NONE

=> s 124

SAMPLE SEARCH INITIATED 01:11:27 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 303 TO ITERATE

100.0% PROCESSED 303 ITERATIONS 1 ANSWERS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 5016 TO 7104
 PROJECTED ANSWERS: 1 TO 80

L25 1 SEA SSS SAM L24

=> s 124 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
 FULL SEARCH INITIATED 01:11:34 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 6201 TO ITERATE

100.0% PROCESSED 6201 ITERATIONS 18 ANSWERS
 SEARCH TIME: 00.00.01

L26 18 SEA SSS FUL L24

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	166.76	605.98
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-12.48

FILE 'REGISTRY' ENTERED AT 01:11:38 ON 12 MAY 2004
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9
 DICTIONARY FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
 information enter HELP PROP at an arrow prompt in the file or refer
 to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> s l26/thu

'THU' IS NOT A VALID CROSSOVER QUALIFIER FOR L26

Answer sets created in a different file may be field qualified with a
 limited set of qualifiers. Enter HELP CROSSOVER at an arrow prompt
 (=>) for specific information.

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.42	606.40

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-12.48

FILE 'HCAPLUS' ENTERED AT 01:11:52 ON 12 MAY 2004

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FILE COVERS 1907 - 12 May 2004 VOL 140 ISS 20

FILE LAST UPDATED: 10 May 2004 (20040510/ED)

This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> d his

(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

L1 STRUCTURE UPLOADED

L2 25 S L1
L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

L4 13 S L3
L5 1 S L4 AND PRIESTLEY, E?/AU
L6 12 S L4 NOT L5
L7 0 S L6 AND DECICCO, C?/AU
L8 0 S L6 AND HUDYMA, T?/AU
L9 0 S L6 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004

L10 0 S L3

FILE 'REGISTRY' ENTERED AT 00:33:56 ON 12 MAY 2004

L11 STRUCTURE UPLOADED
L12 37 S L11
L13 595 S L11 FULL
L14 148 S L13 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:47:52 ON 12 MAY 2004

L15 5 S L14/THU
L16 1 S L15 AND PRIESTLEY, E?/AU
L17 0 S L16 NOT L5
L18 4 S L15 NOT L16
L19 1 S L15 AND DECICCO, C?/AU
L20 0 S L19 NOT L16
L21 0 S L18 AND HYDYMA, T?/AU
L22 0 S L18 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:50:07 ON 12 MAY 2004

L23 0 S L14

FILE 'REGISTRY' ENTERED AT 00:54:59 ON 12 MAY 2004

L24 STRUCTURE UPLOADED
L25 1 S L24
L26 18 S L24 FULL

FILE 'REGISTRY' ENTERED AT 01:11:38 ON 12 MAY 2004

FILE 'HCAPLUS' ENTERED AT 01:11:52 ON 12 MAY 2004

=> s 126/thu

8 L26
591649 THU/RL
L27 3 L26/THU
(L26 (L) THU/RL)

=> d 127, ibib abs fhitr, 1-3

L27 ANSWER 1 OF 3 HCAPLUS. COPYRIGHT 2004 ACS on STN

Full Citing
Text References

ACCESSION NUMBER: 2003:633749 HCAPLUS
DOCUMENT NUMBER: 139:180347
TITLE: Preparation of histogranin-like peptides and non-peptides
INVENTOR(S): Lemaire, Simon; Bernatchez-Lemaire, Irma; Le, Hoang-Tanh
PATENT ASSIGNEE(S): University of Ottawa, Can.

SOURCE: PCT Int. Appl., 59 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003066673	A1	20030814	WO 2003-CA148	20030205
WO 2003066673	C1	20031204		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003176329	A1	20030918	US 2002-68905	20020207
PRIORITY APPLN. INFO.: US 2002-68905 A 20020207				
OTHER SOURCE(S): MARPAT 139:180347				
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to new basic amino acid derivs. I, II and III [A is H, alkyl, or hydroxyalkyl; B is guanidinoalkyl, 4-imidazolylalkyl, aminoalkyl, p-aminophenylalkyl, p-guanidinophenylalkyl, or 4-pyridinylalkyl; D is CO, CO-alkylene, or alkylene; E is a single bond or alkylene; Z is NH₂, amino groups, OH, alkoxy, benzyloxy, or halobenzyl; R1-R5 are independently H or various substituents] and to their prepn. and use in treatment of pain. The compds. have histogranin-like antinociceptive, morphine potentiating and COX-2 induction modulating activities. Thus, cyclo[Gly-(p-chloro)Phe-Tyr-D-Arg] (I-1) was prepd. on an oxime resin using tert-butoxycarbonyl (Boc) protection and cleaved from the resin using intrachain aminolysis in the presence of AcOH and diisopropylethylamine. I-1 showed AD₅₀ = 0.17 nmol/mouse and an analgesic potency ratio of 135 relative to histogranin in a mouse writhing pain assay.

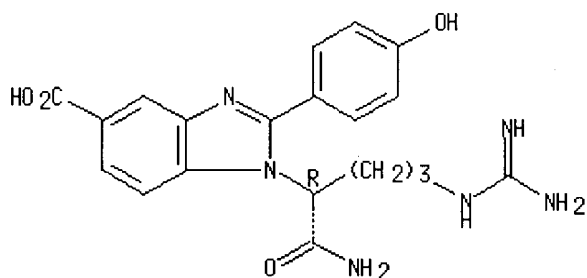
IT 573720-54-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); **THU** (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of histogranin-like peptides and non-peptides)

RN 573720-54-4 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 1-[(1R)-1-(aminocarbonyl)-4-[(aminoiminomethyl)amino]butyl]-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2003:203407 HCAPLUS
 DOCUMENT NUMBER: 138:238181
 TITLE: Preparation of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C
 INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito
 PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
 SOURCE: U.S. Pat. Appl. Publ., 406 pp., Cont.-in-part of Appl. No. PCT/JP00/09181.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003050320	A1	20030313	US 2001-939374	20010824
WO 2001047883	A1	20010705	WO 2000-JP9181	20001222
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG JP 2001247550 A2 20010911 JP 2000-391904 20001225				
PRIORITY APPLN. INFO.:			JP 1999-369008	A 19991227
			WO 2000-JP9181	A2 20001222
			JP 2000-391904	A 20001225
			JP 2001-193786	A 20010626

OTHER SOURCE(S): MARPAT 138:238181
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5,

G6, G8, G9 = C, N; G7 = O, S, CR7, etc.; R1-R4 = H, NO2, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = Ph, cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, CN, etc.; R7 = H, alkyl] are prepd. and formulated. Compds. I showed HCV polymerase inhibitory activity (data given). E.g., a multi-step synthesis of II.HCl, starting from 2-bromo-5-nitrotoluene and Me 2-(2-fluoro-4-hydroxyphenyl)-1-cyclohexylbenzimidazole-5-carboxylate, was given.

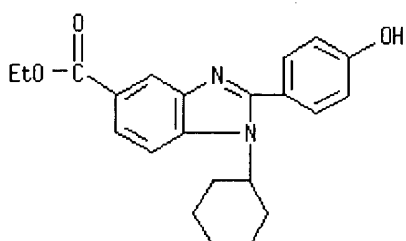
IT 347165-36-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C)

RN 347165-36-0 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-(4-hydroxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)



L27 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2001:489367 HCAPLUS
 DOCUMENT NUMBER: 135:76874
 TITLE: Preparation of heterocyclic compounds as remedies for hepatitis C
 INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito
 PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
 SOURCE: PCT Int. Appl., 438 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

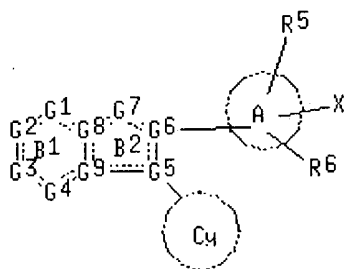
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1162196	A1	20011212	EP 2000-987728	20001222
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000008525	A	20020102	BR 2000-8525	20001222

TR 200103147	T1	20020621	TR 2001-200103147	20001222
NZ 514403	A	20021025	NZ 2000-514403	20001222
AU 763356	B2	20030717	AU 2001-24017	20001222
RU 2223761	C2	20040220	RU 2001-126283	20001222
NO 2001004134	A	20011022	NO 2001-4134	20010824
US 2003050320	A1	20030313	US 2001-939374	20010824
ZA 2001007870	A	20020925	ZA 2001-7870	20010928

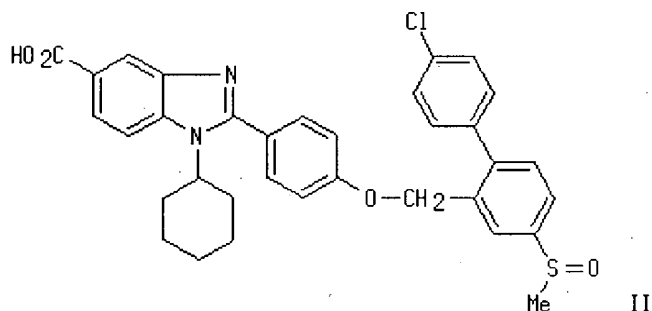
PRIORITY APPLN. INFO.:

JP 1999-369008	A	19991227
WO 2000-JP9181	W	20001222
JP 2000-391904	A	20001225
JP 2001-193786	A	20010626

OTHER SOURCE(S): MARPAT 135:76874
GI



I



II

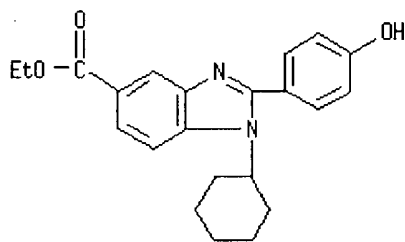
AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, etc.; R1 - R4 = H, nitro, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = C3-C8 cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, cyano, etc.] are prepd. The benzimidazole deriv. II in vitro showed IC50 of 0.011 μ M against hepatitis C virus polymerase. A formulation is given.

IT 347165-36-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of heterocyclic compds. as remedies for hepatitis C)

RN 347165-36-0 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-(4-hydroxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	18.99	625.39
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.08	-14.56

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FILE COVERS 1907-1966
 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

L1 STRUCTURE UPLOADED
 L2 25 S L1
 L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

L4 13 S L3
 L5 1 S L4 AND PRIESTLEY, E?/AU
 L6 12 S L4 NOT L5
 L7 0 S L6 AND DECICCO, C?/AU
 L8 0 S L6 AND HUDYMA, T?/AU
 L9 0 S L6 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:33:48, ON 12 MAY 2004

L10 0 S L3

FILE 'REGISTRY' ENTERED AT 00:33:56 ON 12 MAY 2004

L11 STRUCTURE UPLOADED

L12 37 S L11

L13 595 S L11 FULL

L14 148 S L13 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:47:52 ON 12 MAY 2004

L15 5 S L14/THU

L16 1 S L15 AND PRIESTLEY, E?/AU

L17 0 S L16 NOT L5

L18 4 S L15 NOT L16

L19 1 S L15 AND DECICCO, C?/AU

L20 0 S L19 NOT L16

L21 0 S L18 AND HYDYMA, T?/AU

L22 0 S L18 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:50:07 ON 12 MAY 2004

L23 0 S L14

FILE 'REGISTRY' ENTERED AT 00:54:59 ON 12 MAY 2004

L24 STRUCTURE UPLOADED

L25 1 S L24

L26 18 S L24 FULL

FILE 'REGISTRY' ENTERED AT 01:11:38 ON 12 MAY 2004

FILE 'HCAPLUS' ENTERED AT 01:11:52 ON 12 MAY 2004

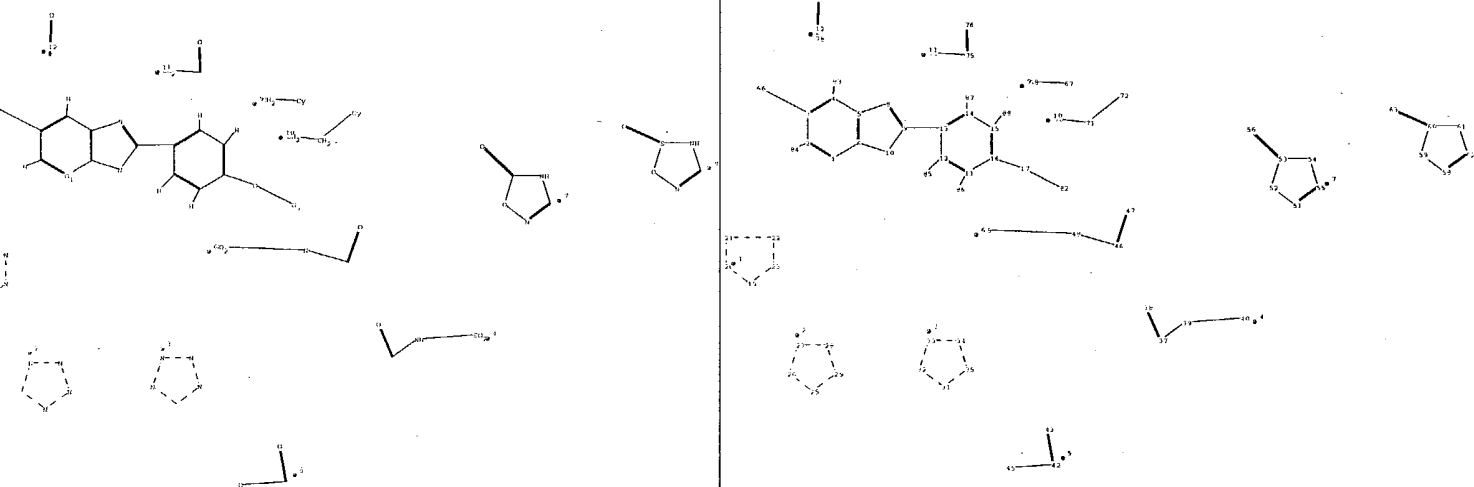
L27 3 S L26/THU

FILE 'CAOLD' ENTERED AT 01:12:49 ON 12 MAY 2004

=> s 126

L28 0 L26

=>



in nodes :
 17 37 38 39 40 42 43 45 46 47 48 49 56 63 66 67 68 70 71 72 74 75 76
 78 79 82 83 84 85 86 87 88

g nodes :
 1 2 3 4 5 6 8 9 10 11 12 13 14 15 16 19 20 21 22 23 25 26 27 28 29
 31 32 33 34 35 51 52 53 54 55 58 59 60 61 62

in bonds :
 2-84 3-66 4-83 9-13 11-86 12-85 14-87 15-88 16-17 17-82 37-38 37-39 39-40
 42-43 42-45 46-47 46-48 48-49 53-56 60-63 67-68 70-71 71-72 74-75 75-76 78-79

g bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 5-8 6-10 8-9 9-10 11-12 11-16 12-13 13-14 14-15
 15-16 19-20 19-23 20-21 21-22 22-23 25-26 25-29 26-27 27-28 28-29 31-32 31-35
 32-33 33-34 34-35 51-52 51-55 52-53 53-54 54-55 58-59 58-62 59-60 60-61 61-62

ct/norm bonds :
 1-2 1-6 2-3 2-84 3-4 3-66 4-5 4-83 5-6 5-8 6-10 8-9 9-10 9-13 11-86 12-85
 14-87 15-88 16-17 17-82 19-20 19-23 20-21 21-22 22-23 25-26 25-29 26-27 27-28
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 48-49 51-52 51-55 52-53 53-54 53-56 54-55 58-59 58-62 59-60 60-61 60-63 61-62
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malized bonds :
 11-12 11-16 12-13 13-14 14-15 15-16

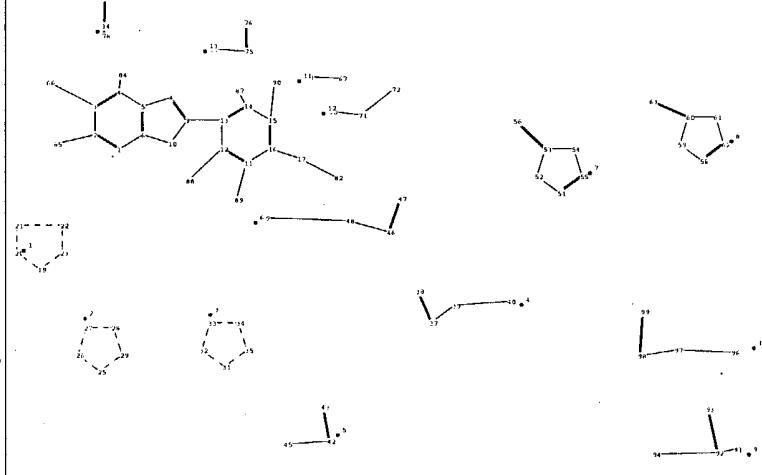
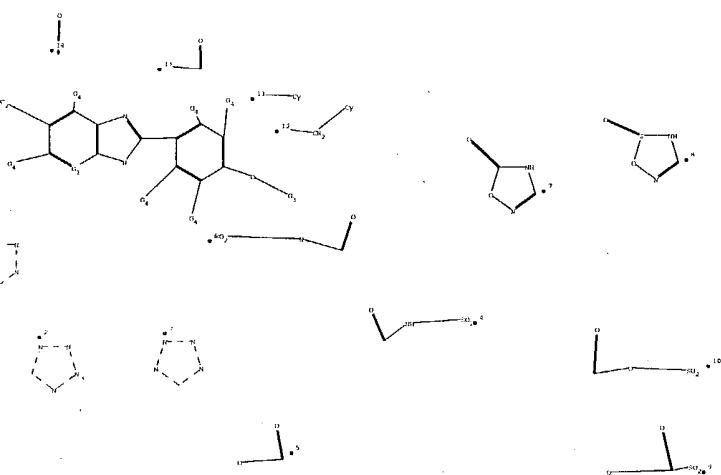
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 containing 1 : 11 : 51 : 58 :

C,N
 [*1],[*2],[*3],[*4],[*5],[*6],[*7],[*8]

Cy,[*9],[*10],[*11],[*12]

ch level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
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 25:Atom

26:Atom 27:Atom 28:Atom 29:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom
37:CLASS 38:CLASS 39:CLASS 40:CLASS 42:CLASS 43:CLASS 45:CLASS 46:CLASS 47:CLASS
48:CLASS 49:CLASS 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:CLASS 58:Atom 59:Atom
60:Atom 61:Atom 62:Atom 63:CLASS 66:CLASS 67:Atom 68:CLASS 70:CLASS 71:CLASS
72:Atom 74:CLASS 75:CLASS 76:CLASS 78:CLASS 79:CLASS 82:CLASS 83:CLASS 84:CLASS
85:CLASS 86:CLASS 87:CLASS 88:CLASS



main nodes :
 17 37 38 39 40 42 43 45 46 47 48 49 56 63 66 67 68 70 71 72 74 75 76
 78 79 82 84 85 87 88 89 90 91 92 93 94 96 97 98 99
 hanging nodes :
 1 2 3 4 5 6 8 9 10 11 12 13 14 15 16 19 20 21 22 23 25 26 27 28 29
 31 32 33 34 35 51 52 53 54 55 58 59 60 61 62
 main bonds :
 2-85 3-66 4-84 9-13 11-89 12-88 14-87 15-90 16-17 17-82 37-38 37-39 39-40
 42-43 42-45 46-47 46-48 48-49 53-56 60-63 67-68 70-71 71-72 74-75 75-76 78-79
 91-92 92-93 92-94 96-97 97-98 98-99
 hanging bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 5-8 6-10 8-9 9-10 11-12 11-16 12-13 13-14 14-15
 15-16 19-20 19-23 20-21 21-22 22-23 25-26 25-29 26-27 27-28 28-29 31-32 31-35
 32-33 33-34 34-35 51-52 51-55 52-53 53-54 54-55 58-59 58-62 59-60 60-61 61-62
 exact/norm bonds :
 1-2 1-6 2-3 2-85 3-4 3-66 4-5 4-84 5-6 5-8 6-10 8-9 9-10 9-13 11-89 12-88
 14-87 15-90 16-17 17-82 19-20 19-23 20-21 21-22 22-23 25-26 25-29 26-27 27-28
 28-29 31-32 31-35 32-33 33-34 34-35 37-38 37-39 39-40 42-43 42-45 46-47 46-48
 48-49 51-52 51-55 52-53 53-54 53-56 54-55 58-59 58-62 59-60 60-61 60-63 61-62
 67-68 70-71 71-72 74-75 75-76 78-79 91-92 92-93 92-94 96-97 97-98 98-99
 normalized bonds :
 11-12 11-16 12-13 13-14 14-15 15-16
 isolated ring systems :
 containing 1 : 11 : 51 : 58 :

C,N

[*1],[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10]

Cy,[*11],[*12],[*13],[*14]

H,F,CH3,NH2

catch level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom
37:CLASS 38:CLASS 39:CLASS 40:CLASS 42:CLASS 43:CLASS 45:CLASS 46:CLASS 47:CLASS
48:CLASS 49:CLASS 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:CLASS 58:Atom 59:Atom
60:Atom 61:Atom 62:Atom 63:CLASS 66:CLASS 67:Atom 68:CLASS 70:CLASS 71:CLASS
72:Atom 74:CLASS 75:CLASS 76:CLASS 78:CLASS 79:CLASS 82:CLASS 84:CLASS 85:CLASS
87:CLASS 88:CLASS 89:CLASS 90:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS 96:CLASS
97:CLASS 98:CLASS 99:CLASS

=> d his

(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

L1 STRUCTURE UPLOADED

L2 25 S L1

L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

L4 13 S L3

L5 1 S L4 AND PRIESTLEY, E?/AU

L6 12 S L4 NOT L5

L7 0 S L6 AND DECICCO, C?/AU

L8 0 S L6 AND HUDYMA, T?/AU

L9 0 S L6 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004

L10 0 S L3

FILE 'REGISTRY' ENTERED AT 00:33:56 ON 12 MAY 2004

L11 STRUCTURE UPLOADED

L12 37 S L11

L13 595 S L11 FULL

L14 148 S L13 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:47:52 ON 12 MAY 2004

L15 5 S L14/THU

L16 1 S L15 AND PRIESTLEY, E?/AU

L17 0 S L16 NOT L5

L18 4 S L15 NOT L16

L19 1 S L15 AND DECICCO, C?/AU

L20 0 S L19 NOT L16

L21 0 S L18 AND HYDYMA, T?/AU

L22 0 S L18 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:50:07 ON 12 MAY 2004

=> s 114

L23 0 L14

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
 NEWS 2 "Ask CAS" for self-help around the clock
 NEWS 3 JAN 27 Source of Registration (SR) information in REGISTRY updated
 and searchable
 NEWS 4 JAN 27 A new search aid, the Company Name Thesaurus, available in
 CA/Caplus
 NEWS 5 FEB 05 German (DE) application and patent publication number format
 changes
 NEWS 6 MAR 03 MEDLINE and LMedLINE reloaded
 NEWS 7 MAR 03 MEDLINE file segment of TOXCENTER reloaded
 NEWS 8 MAR 03 FRANCEPAT now available on STN
 NEWS 9 MAR 29 Pharmaceutical Substances (PS) now available on STN
 NEWS 10 MAR 29 WPIFV now available on STN
 NEWS 11 MAR 29 New monthly current-awareness alert (SDI) frequency in RAPRA
 NEWS 12 APR 26 PROMT: New display field available
 NEWS 13 APR 26 IFIPAT/IFIUDB/IFICDB: New super search and display field
 available
 NEWS 14 APR 26 LITALERT now available on STN
 NEWS 15 APR 27 NLDB: New search and display fields available
 NEWS 16 May 10 PROUSDDR now available on STN
 NEWS 17 May 10 PROUSDDR: One FREE connect hour, per account, in both May
 and June 2004

NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
 MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
 AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
 NEWS HOURS STN Operating Hours Plus Help Desk Availability
 NEWS INTER General Internet Information
 NEWS LOGIN Welcome Banner and News Items
 NEWS PHONE Direct Dial and Telecommunication Network Access to STN
 NEWS WWW CAS World Wide Web Site (general information)

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 specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

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Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9
 DICTIONARY FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
 information enter HELP PROP at an arrow prompt in the file or refer
 to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

=> s l1

SAMPLE SEARCH INITIATED 00:32:07 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 302 TO ITERATE

100.0% PROCESSED 302 ITERATIONS 25 ANSWERS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**

PROJECTED ITERATIONS: 4998 TO 7082

PROJECTED ANSWERS: 200 TO 800

L2 25 SEA SSS SAM L1

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 00:32:12 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 6058 TO ITERATE

100.0% PROCESSED 6058 ITERATIONS 447 ANSWERS
 SEARCH TIME: 00.00.01

L3 447 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	168.44	168.65

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

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FILE COVERS 1907 - 12 May 2004 VOL 140 ISS 20
FILE LAST UPDATED: 10 May 2004 (20040510/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4 13 L3

=> s 14 and priestley, e?/au

64 PRIESTLEY, E?/AU

L5 1 L4 AND PRIESTLEY, E?/AU

=> d 15, ibib abs fhitr, 1

L5 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing
References

ACCESSION NUMBER: 2003:261620 HCAPLUS
DOCUMENT NUMBER: 138:287673
TITLE: Preparation of phenylbenzimidazole compounds useful for treating hepatitis C virus
INVENTOR(S): Priestley, Eldon Scott; Decicco, Carl P.; Hudyma, Thomas W.; Zheng, Xiaofan
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

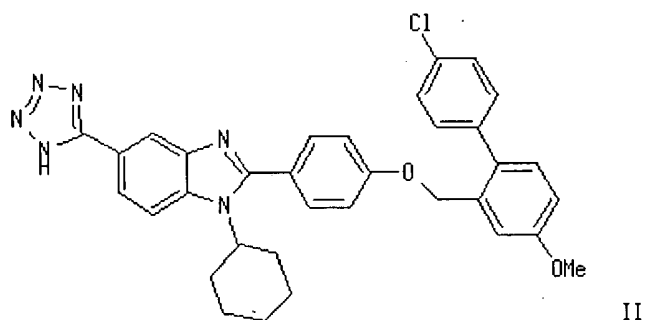
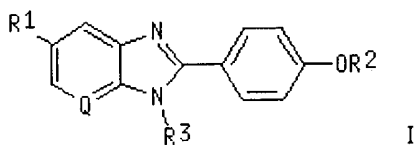
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003026587	A2	20030403	WO 2002-US30989	20020926
WO 2003026587	A3	20031106		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003134853 A1 20030717 US 2002-259041 20020926
US 2004067976 A1 20040408 US 2003-648873 20030827
PRIORITY APPLN. INFO.: US 2001-324874P P 20010926
US 2002-259041 B1 20020926

OTHER SOURCE(S): MARPAT 138:287673

GI



AB Compds. of formula I [Q = CH, N; R1 = tetrazolyl, MeCONHSO2, PhCONHSO2, etc.; R2 = CH2-aryl, CHPh2, etc.; R3 = cycloalkyl] are prepd. which are useful in treating viral hepatitis C. Thus, II was prepd. and had an IC50 of 0.14 μ M against HCV NS5B RdRp (RNA-dependent RNA polymerase).

IT 503857-56-5P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of phenylbenzimidazole compds. for treating hepatitis C viral infection)

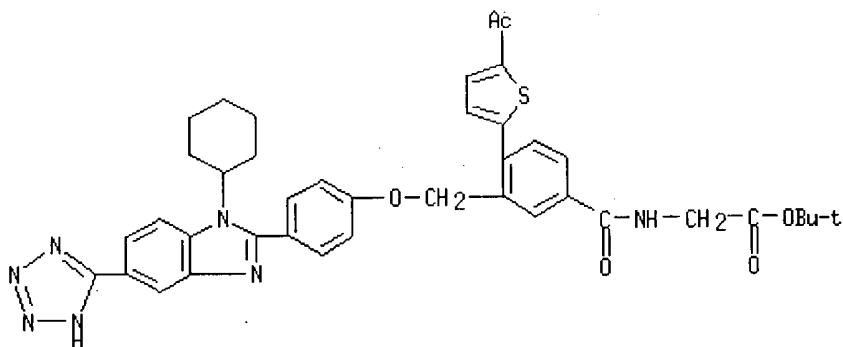
RN 503857-56-5 HCAPLUS

CN Glycine, N-[4-(5-acetyl-2-thienyl)-3-[[4-[1-cyclohexyl-5-(1H-tetrazol-5-yl)-1H-benzimidazol-2-yl]phenoxy]methyl]benzoyl]-, 1,1-dimethylethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 503857-55-4

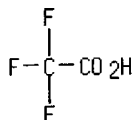
CMF C40 H41 N7 O5 S



CM 2

CRN 76-05-1

CMF C2 H F3 O2



=> d his

(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

L1 STRUCTURE UPLOADED

L2 25 S L1

L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

L4 13 S L3

L5 1 S L4 AND PRIESTLEY, E?/AU

=> s 14 not 15

L6 12 L4 NOT L5

=> s 16 and decicco, c?/au

125 DECICCO, C?/AU

L7 0 L6 AND DECICCO, C?/AU

=> s 16 and hudyma, t?/au

45 HUDYMA, T?/AU

L8 0 L6 AND HUDYMA, T?/AU

=> s 16 and zheng, x?/au

3518 ZHENG, X?/AU

L9 0 L6 AND ZHENG, X?/AU

=> d 16, ibib abs fhitstr, 1-12

L6 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2003:981461 HCAPLUS

DOCUMENT NUMBER: 140:246106

TITLE: Non-nucleoside inhibitors of the hepatitis C virus NS5B polymerase: discovery and preliminary SAR of benzimidazole derivatives

AUTHOR(S): Beaulieu, Pierre L.; Bos, Michael; Bousquet, Yves; Fazal, Gulrez; Gauthier, Jean; Gillard, James; Goulet, Sylvie; LaPlante, Steven; Poupart, Marc-Andre; Lefebvre, Sylvain; McKercher, Ginette; Pellerin, Charles; Austel, Volkhard; Kukolj, George

CORPORATE SOURCE: Department of Chemistry, Research and Development, Boehringer Ingelheim (Canada) Ltd., Laval, QC, H7S 2G5, Can.

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(1), 119-124

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Benzimidazole 5-carboxamide derivs. from a combinatorial screening library were discovered as specific inhibitors of the NS5B polymerase of the hepatitis C virus (HCV). Initial hit-to-lead activities taking advantage of high-throughput parallel synthetic techniques, identified a 1,2-disubstituted benzimidazole 5-carboxylic acid scaffold as the min. core for biol. activity. Potent analogs in this series inhibit the polymerase at low micromolar concns. and provide an attractive 'drug-like' lead structure for further optimization and the development of potential HCV therapeutics.

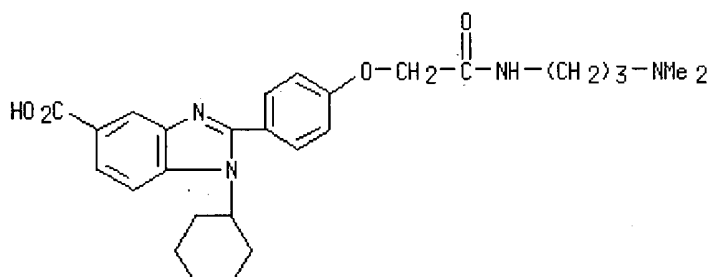
IT 390815-16-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(discovery and preliminary SAR of benzimidazole derivs. as inhibitors of hepatitis C virus NS5B polymerase)

RN 390815-16-4 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[4-[2-[[3-(dimethylamino)propyl]amino]-2-oxoethoxy]phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2003:319709 HCAPLUS
DOCUMENT NUMBER: 138:338144
TITLE: Preparation of 2-phenyl benzimidazoles and imidazo-[4,5]pyridines as Cds1/Chk2-inhibitors and adjuvants to chemotherapy or radiation therapy in the treatment of cancer
INVENTOR(S): Arienti, Kristen L.; Axe, Frank U.; Breitenbucher, J. Guy; Huang, Liming; Lee, Alice; McClure, Kelly J.
PATENT ASSIGNEE(S): Ortho-McNeil Pharmaceutical, Inc., USA
SOURCE: PCT Int. Appl., 144 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003032984	A1	20030424	WO 2002-US33371	20021018
WO 2003032984	C1	20031120		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,

Maybe = make sure then use

102(a) promiscuous & 103(a)

PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
 UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
 TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
 CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
 PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
 NE, SN, TD, TG

US 2003176438 A1 20030918 US 2002-273487 20021018

NO 2003002759 A 20030818 NO 2003-2759 20030617

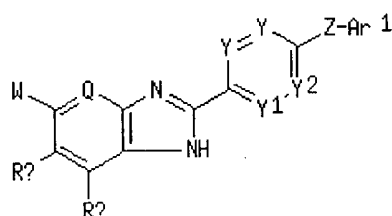
PRIORITY APPLN. INFO.:

US 2001-330304P P 20011019

WO 2002-US33371 W 20021018

OTHER SOURCE(S): MARPAT 138:338144

GI



I

check

AB 2-Aryl-substituted benzimidazoles and imidazo[4,5]pyridines (shown as I; e.g. 2-[4-(4-chlorophenoxy)phenyl]-1H-benzimidazole-5-carboxylic acid amide (II)) are disclosed as inhibitors of Cds1 and useful as adjuvants to chemotherapy or radiation therapy in the treatment of cancer. For I: W is COOH, -C(O)NHR1, or -SO2NHR1 (R1 is H or C1-4alkyl); Q is N or CH; Ra and Rb are H or halogen; Y, Y1 and Y2 = N and C-Rc with the proviso that 0, 1 or 2 of Y, Y1 and Y2 are N and at least 2 of Rc must be H; Rc = -H, -OH, -C1-6alkyl, -SCF3, halo, -CF3 and -OCF3; Z = O, S, SO, SO2, SO2NR2, NR2SO2, NH, CONR2, piperazinediyl or a covalent bond; R2 is H or C1-4alkyl; Ar1 is an arom. group as defined in the claims. IC50 values are reported for inhibition of human Cds1 checkpoint kinase by 103 examples of I, e.g. 3 nM for 2-[4-(4-chloro-3-trifluoromethylphenoxy)phenyl]-1H-benzimidazole-5-carboxylic acid amide. Addnl. studies were (i) detn. of the effect of II on tumor cell line clonogenic survival, (ii) effect of II on tumor growth in murine xenograft models, (iii) detn. of the effect of 14 examples of I on radiation-induced apoptosis in isolated primary cells, and (iv) detn. of the effect of II on radiation-induced apoptosis in splenocytes in vivo. Although the methods of prepn. are not claimed, ~100 example preps. are included.

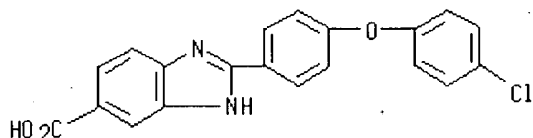
IT 516480-80-1P, 2-[4-(4-Chlorophenoxy)phenyl]-1H-benzimidazole-5-carboxylic acid

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; prepn. of benzimidazoles and imidazopyridines as Cds1/Chk2-inhibitors and adjuvants to chemotherapy or radiation therapy in treatment of cancer)

RN 516480-80-1 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(4-chlorophenoxy)phenyl]- (9CI)
 (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2003:203407. HCAPLUS
 DOCUMENT NUMBER: 138:238181
 TITLE: Preparation of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C
 INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito
 PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
 SOURCE: U.S. Pat. Appl. Publ., 406 pp., Cont.-in-part of Appl. No. PCT/JP00/09181.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

check = 1022 date good

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003050320	A1	20030313	US 2001-939374	20010824
WO 2001047883	A1	20010705	WO 2000-JP9181	20001222
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG JP 2001247550 A2 20010911 JP 2000-391904 20001225				
PRIORITY APPLN. INFO.: JP 1999-369008 A 19991227 WO 2000-JP9181 A2 20001222 JP 2000-391904 A 20001225 JP 2001-193786 A 20010626				
OTHER SOURCE(S): MARPAT 138:238181 GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2; G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, S, CR7, etc.; R1-R4 = H, NO2, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = Ph, cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, CN, etc.; R7 = H, alkyl] are prepd. and formulated. Compds. I showed HCV polymerase inhibitory activity (data

given). E.g., a multi-step synthesis of II.HCl, starting from 2-bromo-5-nitrotoluene and Me 2-(2-fluoro-4-hydroxyphenyl)-1-cyclohexylbenzimidazole-5-carboxylate, was given.

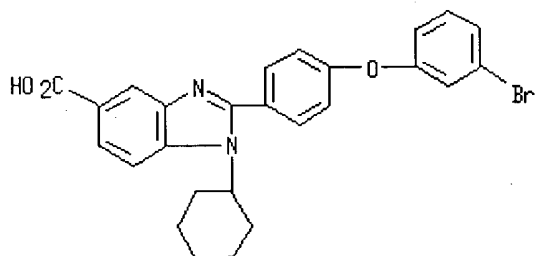
IT 347165-35-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C)

RN 347165-35-9 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(3-bromophenoxy)phenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)



L6 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full
Text

Citing
References

ACCESSION NUMBER: 2003:5773 HCAPLUS

DOCUMENT NUMBER: 138:66657

TITLE: Fused cyclic compounds and medicinal use thereof

INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito

PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan

SOURCE: PCT Int. Appl., 603 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003000254	A1	20030103	WO 2002-JP6405	20020626
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
JP 2003212846	A2	20030730	JP 2002-185241	20020625
BR 2002005684	A	20030617	BR 2002-5684	20020626
EP 1400241	A1	20040324	EP 2002-743728	20020626
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
US 2004082635	A1	20040429	US 2003-344997	20030218
NO 2003000832	A	20030422	NO 2003-832	20030221

PRIORITY APPLN. INFO.:

JP 2001-193786

A 20010626

JP 2001-351537

A 20011116

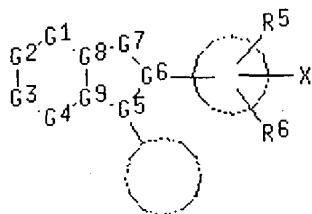
WO 2002-JP6405

W 20020626

OTHER SOURCE(S):

MARPAT 138:66657

GI



I

AB Fused cyclic compds. represented by the following general formula [I] or pharmaceutically acceptable salts thereof and remedies for hepatitis C contg. these compds.: I wherein each symbol is as defined in the description. Because of having an effect against hepatitis C virus (HVC) based on an HCV polymerase inhibitory effect, these compds. are useful as remedies or preventives for hepatitis C.

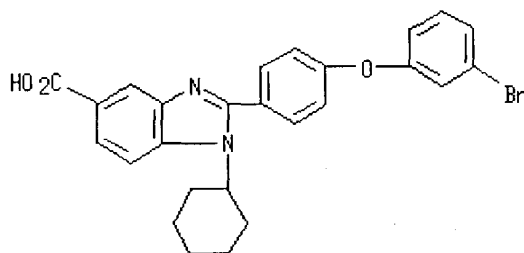
IT 347165-35-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(fused cyclic compds. as hepatitis C virus polymerase inhibitors and antiviral agents)

RN 347165-35-9 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(3-bromophenoxy)phenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

27

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER:

2002:51438 HCAPLUS

DOCUMENT NUMBER:

136:118447

TITLE:

Preparation of benzimidazolecarboxylates and related compounds as viral polymerase inhibitors

INVENTOR(S):

Beaulieu, Pierre Louis; Fazal, Gulrez; Gillard, James; Kukolj, George; Austel, Volkhard

PATENT ASSIGNEE(S):

Boehringer Ingelheim (Canada) Ltd., Can.

SOURCE:

PCT Int. Appl., 322 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

EXPAND

LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

(1,5)-Biphenyl-4-carboxamide
4-(4-ethoxyphenyl)-5-
(1H-tetrazol-5-yl)-
1H-benzimidazol-2-yl
3-fluorophenyl
methyl-N,N
dimethyl.

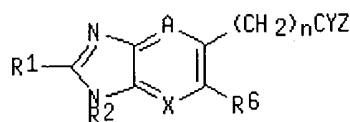
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004425	A2	20020117	WO 2001-CA989	20010704
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002065418	A1	20020530	US 2001-898297	20010703
US 6448281	B2	20020910		
EP 1301487	A2	20030416	EP 2001-951274	20010704
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004502761	T2	20040129	JP 2002-509292	20010704
US 6479508	B1	20021112	US 2001-995099	20011127
WO 2002070739	A2	20020912	WO 2002-CA323	20020306
WO 2002070739	A3	20030530		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1370682	A2	20031217	EP 2002-712681	20020306
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2003232816	A1	20031218	US 2002-238282	20020910

PRIORITY APPLN. INFO.:

US 2000-216084P P 20000706
 US 2001-274374P P 20010308
 US 2001-281343P P 20010405
 US 2001-898297 A3 20010703
 WO 2001-CA989 W 20010704
 US 2001-995099 A3 20011127
 WO 2002-CA323 W 20020306

OTHER SOURCE(S):
 GI

MARPAT 136:118447



AB Title compds. [I; X = CH, N; Y = O, S; Z = OH, NH₂, NMe₃, NHR₃, OR₃, 5-6 membered (substituted) heterocyclyl; A = N, COR₇, CR₅; R₅ = H, halo, alkyl; R₇ = H, alkyl; X and A are not both N; R₆ = H, halo, alkyl, OR₇; R₇ = H, alkyl; R₁ = (substituted) hetero(bi)cyclyl, Ph, phenylalkyl, alkenyl, phenylalkenyl, cycloalkyl, alkyl, CF₃; R₂ = (substituted) alkyl,

cycloalkyl, cycloalkylalkyl, bicycloalkyl, adamantyl, Ph, pyridyl; R3 = H, alkyl, cycloalkyl, cycloalkylalkyl, aryl, arylalkyl, alkenyl, cycloalkylalkenyl, arylalkenyl, dialkylamino, heterocyclyl, etc.; n = 0, 1], were prepd. Thus, Me 3-amino-4-cyclohexylaminobenzoate (prepn. given), 2-pyridinecarboxaldehyde, and Oxone were stirred in DMF to give 80% Et 1-cyclohexyl-2-pyridin-2-yl-1H-benzimidazole-5-carboxylate, which was sapond. with aq. NaOH in MeOH to give 91% 1-cyclohexyl-2-pyridin-2-yl-1H-benzimidazole-5-carboxylic acid. The latter inhibited hepatitis C virus RNA dependent polymerase (NS5B) with IC50 = 1-5 μ M.

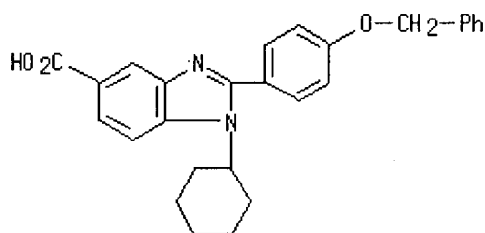
IT 347166-09-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzimidazolecarboxylates and related compds. as viral polymerase inhibitors)

RN 347166-09-0 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2001:489367 HCAPLUS
 DOCUMENT NUMBER: 135:76874
 TITLE: Preparation of heterocyclic compounds as remedies for hepatitis C
 INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito
 PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
 SOURCE: PCT Int. Appl., 438 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001047883	A1	20010705	WO 2000-JP9181	20001222
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1162196	A1	20011212	EP 2000-987728	20001222

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO

BR 2000008525	A	20020102	BR 2000-8525	20001222
TR 200103147	T1	20020621	TR 2001-200103147	20001222
NZ 514403	A	20021025	NZ 2000-514403	20001222
AU 763356	B2	20030717	AU 2001-24017	20001222
RU 2223761	C2	20040220	RU 2001-126283	20001222
NO 2001004134	A	20011022	NO 2001-4134	20010824
US 2003050320	A1	20030313	US 2001-939374	20010824
ZA 2001007870	A	20020925	ZA 2001-7870	20010928

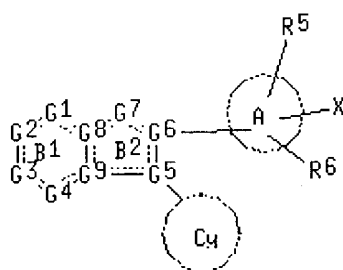
PRIORITY APPLN. INFO.:

JP 1999-369008	A	19991227
WO 2000-JP9181	W	20001222
JP 2000-391904	A	20001225
JP 2001-193786	A	20010626

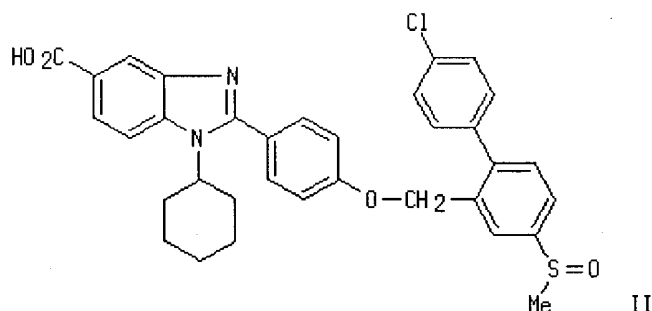
OTHER SOURCE(S):

MARPAT 135:76874

GI



I



II

AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2; G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, etc.; R1 - R4 = H, nitro, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = C3-C8 cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, cyano, etc.] are prepd. The benzimidazole deriv. II in vitro showed IC₅₀ of 0.011 μ M against hepatitis C virus polymerase. A formulation is given.

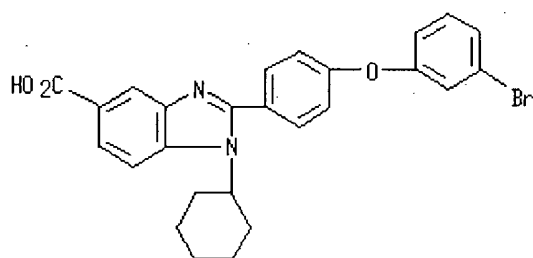
IT 347165-35-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of heterocyclic compds. as remedies for hepatitis C)

RN 347165-35-9 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(3-bromophenoxy)phenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)

Use
Best handled
Se



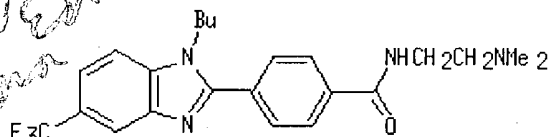
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

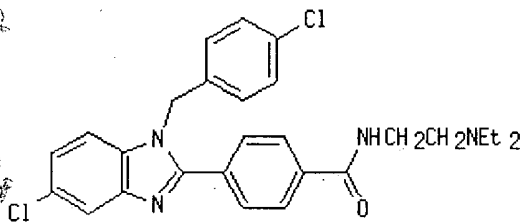
Full Text	Citing References
Full Text	Citing References

ACCESSION NUMBER: 2001:412102 HCAPLUS
DOCUMENT NUMBER: 135:177890
TITLE: Synthesis and antimicrobial activity of some new
2-phenyl-N-substituted carboxamido-1H-benzimidazole
derivatives
AUTHOR(S): Goker, Hakan; Tuncbilek, Meral; Suzen, Sibel; Kus,
Canan; Altanlar, Nurten
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of
Pharmacy, Ankara University, Ankara, 06100, Turk.
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (2001),
334(5), 148-152
CODEN: ARPMAS; ISSN: 0365-6233
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:177890
GI

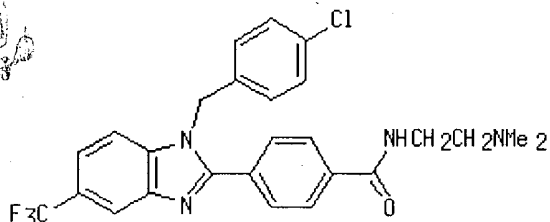
(2001) may have use



I



II



III

AB Some 1H-benzimidazole-carboxamide derivs. were prepd. and their antimicrobial activities against *Staphylococcus aureus*, *Escherichia coli*,

and *Candida albicans* evaluated. Compds. I, II, and III exhibited the best activity against *C. albicans*.

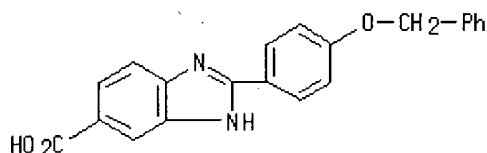
IT **174422-18-5P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and antimicrobial activity of new 2-phenyl-N-substituted carboxamido-1H-benzimidazole derivs.)

RN 174422-18-5 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]- (9CI)
(CA INDEX NAME)

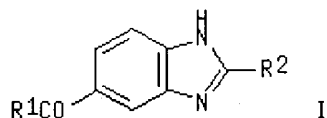


REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 1999:614608 HCAPLUS
DOCUMENT NUMBER: 131:286454
TITLE: Synthesis and antimicrobial activity of some new benzimidazole carboxylates and carboxamides
AUTHOR(S): Ayhan-Kilcigil, Gulgun; Tuncbilek, Meral; Altanlar, Nurten; Goker, Hakan
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Ankara University, Ankara, 06100, Turk.
SOURCE: Farmaco (1999), 54(8), 562-565
CODEN: FRMCE8; ISSN: 0014-827X
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Benzimidazole carboxylates and carboxamides, e.g., I [R1 = MeO, (2-pyridinylmethyl)amino, 4-methylpiperidino, R2 = 2-ClC6H4, 4-ClC6H4, 2,4-Cl2C6H3, 2-MeOC6H4, 4-MeOC6H4, 2-thienyl], were synthesized and evaluated for their antimicrobial activities against *Staphylococcus aureus*, *Escherichia coli*, and *Candida albicans*. Among the investigated compds., I (R1 = MeO, R2 = 2-MeOC6H4) exhibited best activity against *C. albicans*.

IT **246517-85-1P**

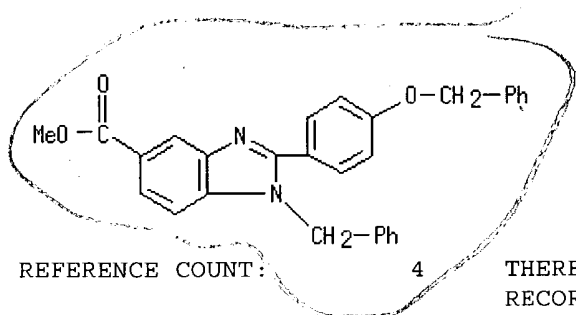
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and antimicrobial activity of benzimidazole carboxylates and carboxamides)

RN 246517-85-1 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]-1-

(phenylmethyl)-, methyl ester (9CI) (CA INDEX NAME)



2 points
difference
Bioisostere?

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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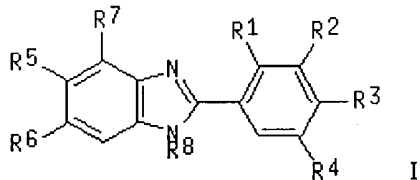
ACCESSION NUMBER: 1999:184240 HCAPLUS
 DOCUMENT NUMBER: 130:209707
 TITLE: Preparation of 2-substituted phenyl-benzimidazole antibacterial agents
 INVENTOR(S): Ohemeng, Kwasi Adomako; Nguyen, Van Nhatton
 PATENT ASSIGNEE(S): Ortho-McNeil Pharmaceutical, Inc., USA
 SOURCE: PCT Int. Appl., 70 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

maybe

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9911627	A1	19990311	WO 1998-US18586	19980904
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 5942532	A	19990824	US 1997-924558	19970905
AU 9893054	A1	19990322	AU 1998-93054	19980904
PRIORITY APPLN. INFO.:			US 1997-924558	19970905
			WO 1998-US18586	19980904

NO EXDm

OTHER SOURCE(S): MARPAT 130:209707
 GI



AB Benzimidazoles I [R1 = H, OH, alkoxy; R2, R3, R4 = H, OH, alkyl, CF3, halo, etc.; R5 = H, amino, amidino; R6 = nitro, C(NHR9):NR10; R7 = H, amino, nitro; R8 = H, Me], antibacterial compds., were prepd. These compds. are effective in inhibiting the action of a bacterial histidine protein kinase and are useful as anti-infective agents against a variety

of bacterial organisms, including organisms which are resistant to other known antibiotics. E.g., 3,4-diaminobenzimidate, prepd. from 3,4-diaminobenzonitrile, was treated with NH_3/EtOH , then with 4-Me $3\text{CC}_6\text{H}_4\text{CHO}$ to give 2-[4-(1,1-dimethylethyl)phenyl]-2H-benzimidazole-5-carboximidamide.

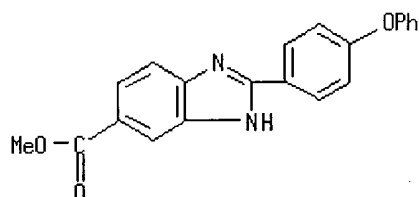
IT **220955-73-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of phenylbenzimidazoles as antibacterial agents)

RN 220955-73-7 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-(4-phenoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)



*103(a)
provide
check
to see if
this
has been
use.
Munich
Bioscience*

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 1998:634393 HCAPLUS

DOCUMENT NUMBER: 129:316174

TITLE: Synthesis of some new benzimidazolecarboxamides and evaluation of their antimicrobial activity

AUTHOR(S): Goker, Hakan; Tuncbilek, Meral; Ayhan, Gulgun; Altanlar, Nurten

CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Ankara University, Ankara, 06100, Turk.

SOURCE: Farmaco (1998), 53(6), 415-420

CODEN: FRMCE8; ISSN: 0014-827X

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of 1,2-disubstituted benzimidazole-5(6)-carboxamides was prepd. and evaluated in vitro for antimicrobial activity against *Staphylococcus aureus*, *Escherichia coli*, and *Candida albicans*. The precursor benzimidazolecarboxylic acids were prepd. via oxidative condensation of diaminobenzoic acids with aldehydes and via several steps over the 2(1H)-benzimidazolones, resp. All acids were converted to their acyl chlorides with SOCl_2 , then amidified with several N,N'-dialkylaminoethyl derivs.

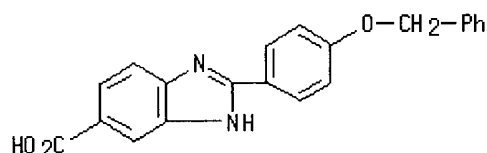
IT **174422-18-5**

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. and bactericidal and fungicidal activity of benzimidazolecarboxamides)

RN 174422-18-5 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 1996:144268 HCAPLUS
 DOCUMENT NUMBER: 124:197998
 TITLE: Synthesis of 1,2-disubstituted benzimidazole-5(6)-carboxamides and evaluation of their antimicrobial activity
 AUTHOR(S): Goeker, Hakan; Tebrizli, Emin; Abbasoglu, Ufuk
 CORPORATE SOURCE: Faculty of Pharmacy, Univ. of Ankara, Tandogan, 06100, Turk.
 SOURCE: Farmaco (1996), 51(1), 53-8
 CODEN: FRMCE8
 PUBLISHER: Societa Chimica Italiana
 DOCUMENT TYPE: Journal
 LANGUAGE: English

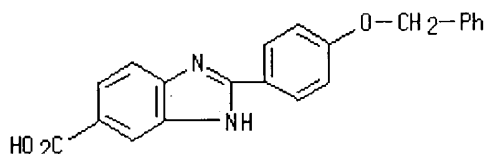
AB Fourteen N'-(N,N-dialkylaminoethyl)-benzimidazole 5(6)- or 5-carboxamides having several substituents on the azole and benzene nuclei were prepd. and evaluated in vitro for antimicrobial activity. The precursor benzimidazolecarboxylic acids were prepd. via oxidative condensation of diaminobenzoic acids and several aldehydes with cupric ion. All carboxamides were prepd. from the corresponding acids and N,N-dialkylethylenediamine. Antibacterial and antifungal activities were detd. as MIC values. Compds. which were prepd. by replacement with bulky alkyl groups on the tert-N benzimidazole atom gave the best results.

IT 174422-18-5P

RL: PRP (Properties); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (synthesis of 1,2-disubstituted benzimidazole-5(6)-carboxamides and evaluation of their antimicrobial activity)

RN 174422-18-5 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(benzyloxy)phenyl]- (9CI)
 (CA INDEX NAME)

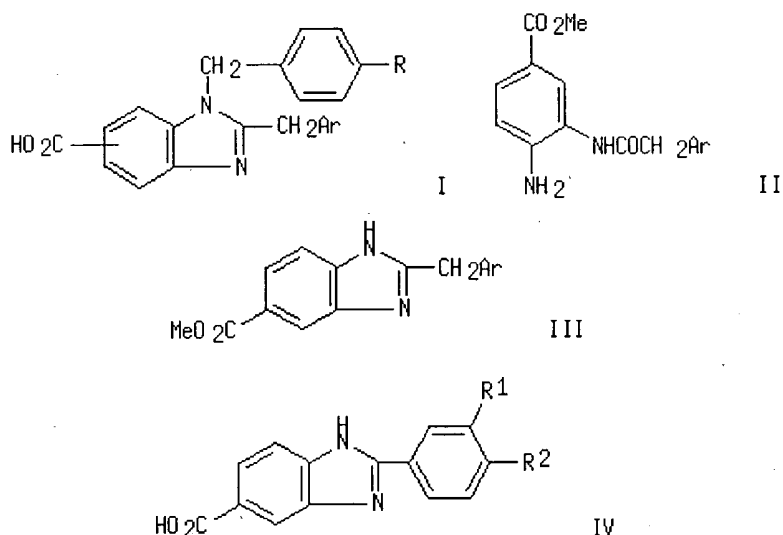


L6 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 1996:38013 HCAPLUS
 DOCUMENT NUMBER: 124:202112
 TITLE: Synthesis of some new benzimidazole-5(6)-carboxylic acids
 AUTHOR(S): Goeker, Hakan; Oelgen, Suereyya; Ertan, Rahmiye; Akguen, Huelya; Oezbey, Sueheyla; Kendi, Engin; Topcu, Guel

CORPORATE SOURCE: Fac. Pharmacy, Ankara Univ., Ankara, 06100, Turk.
 SOURCE: Journal of Heterocyclic Chemistry (1995), 32(6),
 1767-73
 CODEN: JHTCAD; ISSN: 0022-152X
 PUBLISHER: HeteroCorporation
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



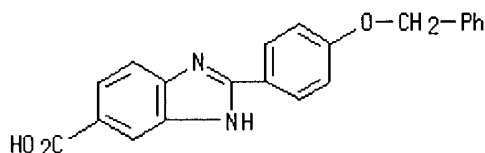
AB The title compds., 1,2-dialkyl-benzimidazole-5(6)-carboxylic acids I (Ar = Ph, 4-MeC₆H₄, 4-ClC₆H₄, 2-BrC₆H₄, OPh, 4-ClC₆H₄O, etc., R = H, F, CO₂H position = 5, 6) were prepd. in four steps; (1) prepn. of mono amide derivs. II by the reaction of Me 3,4-diaminobenzoate and substituted Ph or phenoxyacetic acid chlorides ArCH₂COCl, (2) prepn. of the Me benzimidazolecarboxylates III, with zinc chloride and dry hydrogen chloride gas, (3) alk. hydrolysis of the esters, and (4) substitution of the imidazole ring with benzyl or p-fluorobenzyl bromide, in alkali medium. 2-Aryl-benzimidazole-5(6)-carboxylic acids IV (R₁ = H, OCH₂Ph, OH, R₂ = OCH₂Ph, OH) were prepd. via the oxidative condensation of 3,4-diaminobenzoic acid and arom. aldehydes with cupric ion.

IT 174422-18-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of benzimidazolecarboxylic acids)

RN 174422-18-5 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]- (9CI)
 (CA INDEX NAME)



=> file caold

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
FULL ESTIMATED COST	ENTRY	SESSION
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY	SESSION
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FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004
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FILE COVERS 1907-1966
 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

L1 STRUCTURE UPLOADED
 L2 25 S L1
 L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

L4 13 S L3
 L5 1 S L4 AND PRIESTLEY, E?/AU
 L6 12 S L4 NOT L5
 L7 0 S L6 AND DECICCO, C?/AU
 L8 0 S L6 AND HUDYMA, T?/AU
 L9 0 S L6 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004

=> s 13

L10 0 L3

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

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STRUCTURE FILE UPDATES:    10 MAY 2004    HIGHEST RN 681120-30-9
DICTIONARY FILE UPDATES:  10 MAY 2004    HIGHEST RN 681120-30-9
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TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

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C4 91

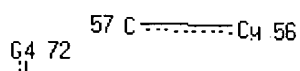
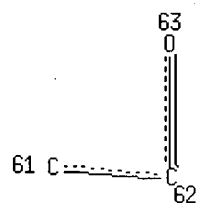
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G4 67
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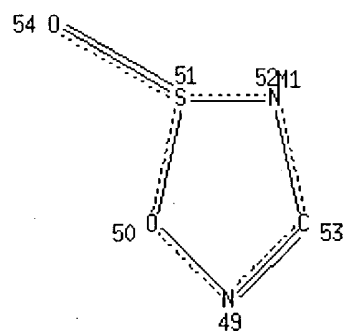


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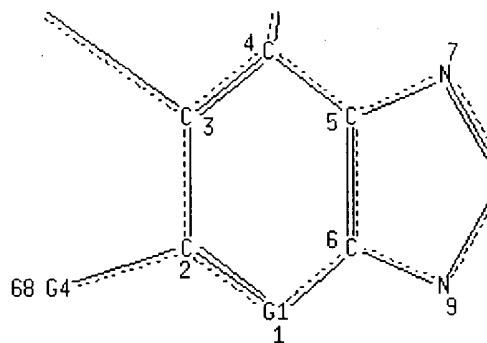
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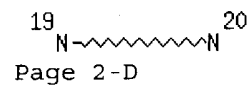
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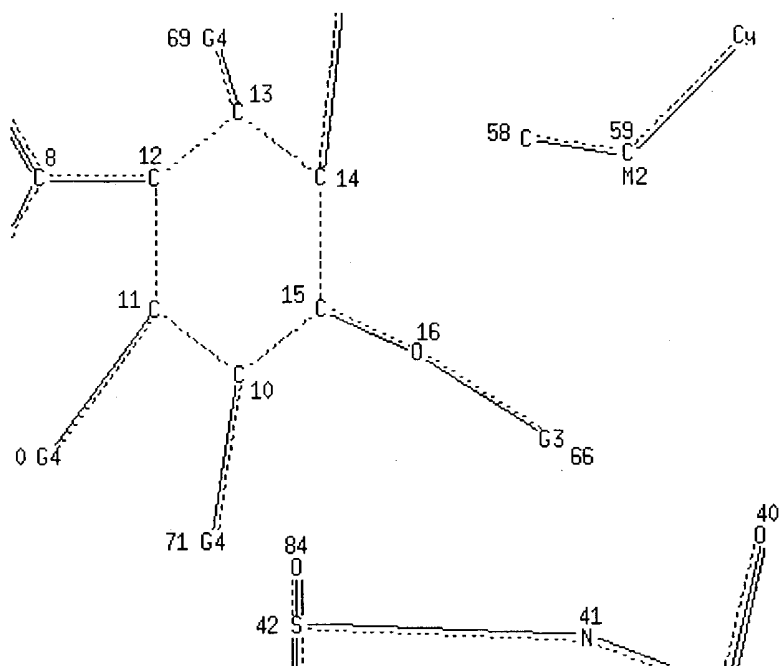
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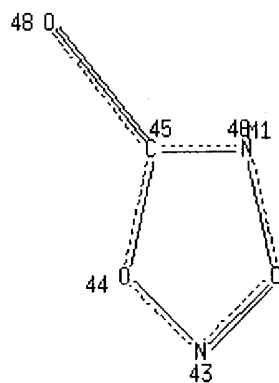
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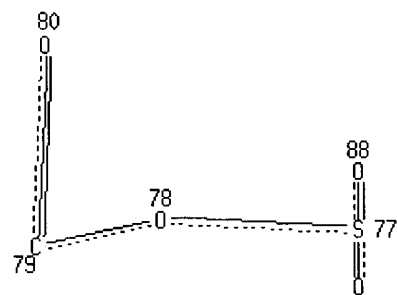
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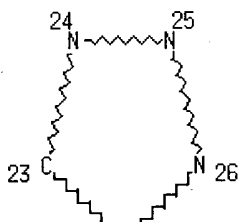
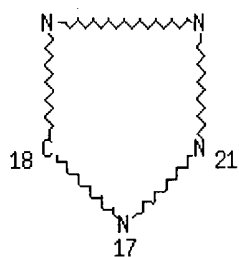
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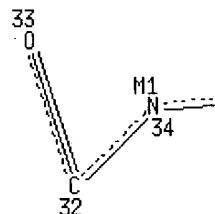
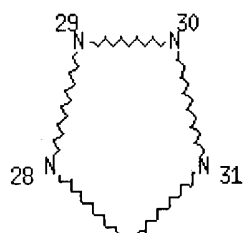
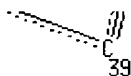
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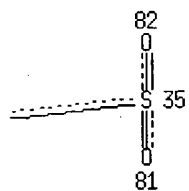
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Page 3-D

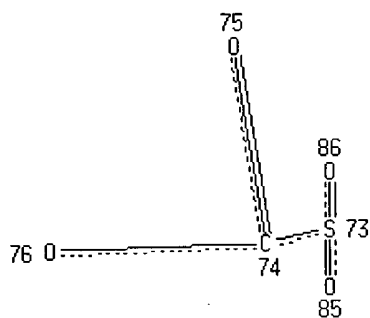


Page 3-E



Page 3-F

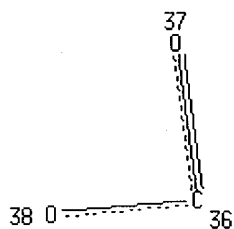
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Page 4-B



Page 4-D



Page 4-E

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VAR G2=18/24/29/35/36/42/47/53/73/77

VAR G3=91/57/58/61/64

VAR G4=92/93/94/95

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HCOUNT	IS M2	AT	59
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GRAPH ATTRIBUTES:
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NUMBER OF NODES IS  95

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STEREO ATTRIBUTES: NONE

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SAMPLE SCREEN SEARCH COMPLETED - 302 TO ITERATE

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100.0% PROCESSED      302 ITERATIONS                      37 ANSWERS
SEARCH TIME: 00.00.01

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FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:   4998 TO    7082
PROJECTED ANSWERS:      376 TO    1104

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L12          37 SEA SSS SAM L11

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THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
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FULL SCREEN SEARCH COMPLETED - 6058 TO ITERATE

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SEARCH TIME: 00.00.01

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L13          595 SEA SSS FUL L11

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=> d his

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(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

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FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

```

```

L1          STRUCTURE UPLOADED

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L2 25 S L1
L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

L4 13 S L3
L5 1 S L4 AND PRIESTLEY, E?/AU
L6 12 S L4 NOT L5
L7 0 S L6 AND DECICCO, C?/AU
L8 0 S L6 AND HUDYMA, T?/AU
L9 0 S L6 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004

L10 0 S L3

FILE 'REGISTRY' ENTERED AT 00:33:56 ON 12 MAY 2004

L11 STRUCTURE UPLOADED
L12 37 S L11
L13 595 S L11 FULL

=> s l13 not l3

L14 148 L13 NOT L3

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	164.66	402.64

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-9.01

FILE 'HCAPLUS' ENTERED AT 00:47:52 ON 12 MAY 2004

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FILE COVERS 1907 - 12 May 2004 VOL 140 ISS 20

FILE LAST UPDATED: 10 May 2004 (20040510/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l14/thu

5 L14
591649 THU/RL
L15 5 L14/THU
(L14 (L) THU/RL)

=> s l15 and priestley, e?/au
 64 PRIESTLEY, E?/AU
 L16 1 L15 AND PRIESTLEY, E?/AU

=> d his

(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

L1 STRUCTURE UPLOADED
 L2 25 S L1
 L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

L4 13 S L3
 L5 1 S L4 AND PRIESTLEY, E?/AU
 L6 12 S L4 NOT L5
 L7 0 S L6 AND DECICCO, C?/AU
 L8 0 S L6 AND HUDYMA, T?/AU
 L9 0 S L6 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004

L10 0 S L3

FILE 'REGISTRY' ENTERED AT 00:33:56 ON 12 MAY 2004

L11 STRUCTURE UPLOADED
 L12 37 S L11
 L13 595 S L11 FULL
 L14 148 S L13 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:47:52 ON 12 MAY 2004

L15 5 S L14/THU
 L16 1 S L15 AND PRIESTLEY, E?/AU

=> s l16 not 15

L17 0 L16 NOT L5

=> d l16, ibib abs fhitr, 1

L16 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
ACCESSION NUMBER:	2003:261620 HCAPLUS
DOCUMENT NUMBER:	138:287673
TITLE:	Preparation of phenylbenzimidazole compounds useful for treating hepatitis C virus
INVENTOR(S):	Priestley, Eldon Scott ; Decicco, Carl P.; Hudyma, Thomas W.; Zheng, Xiaofan
PATENT ASSIGNEE(S):	Bristol-Myers Squibb Company, USA
SOURCE:	PCT Int. Appl., 74 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
<u>PATENT INFORMATION:</u>	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003026587	A2	20030403	WO 2002-US30989	20020926
WO 2003026587	A3	20031106		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

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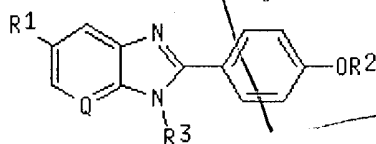
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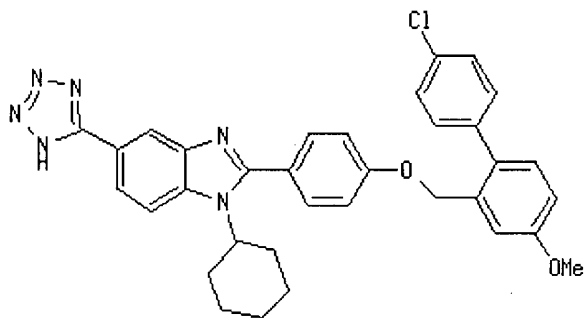
OTHER SOURCE(S):

MARPAT 138:287673

GI



1025904



AB Compds. of formula I [Q = CH, N; R1 = tetrazolyl, MeCONHSO₂, PhCONHSO₂, etc.; R2 = CH₂-aryl, CHPh₂, etc.; R3 = cycloalkyl] are prepd. which are useful in treating viral hepatitis C. Thus, II was prepd. and had an IC₅₀ of 0.14 μM against HCV NS5B RdRp (RNA-dependent RNA polymerase).

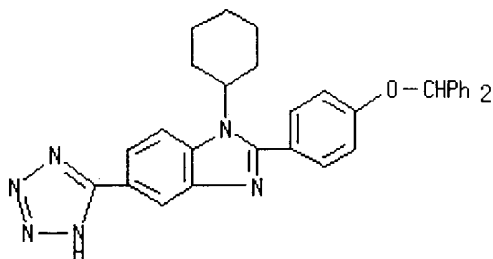
IT 503857-49-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); **THU** (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of phenylbenzimidazole compds. for treating hepatitis C viral infection)

RN 503857-49-6 HCAPLUS

CN 1H-Benzimidazole, 1-cyclohexyl-2-[4-(diphenylmethoxy)phenyl]-5-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

L1 STRUCTURE UPLOADED
L2 25 S L1
L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

L4 13 S L3
L5 1 S L4 AND PRIESTLEY, E?/AU
L6 12 S L4 NOT L5
L7 0 S L6 AND DECICCO, C?/AU
L8 0 S L6 AND HUDYMA, T?/AU
L9 0 S L6 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004

L10 0 S L3

FILE 'REGISTRY' ENTERED AT 00:33:56 ON 12 MAY 2004

L11 STRUCTURE UPLOADED
L12 37 S L11
L13 595 S L11 FULL
L14 148 S L13 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:47:52 ON 12 MAY 2004

L15 5 S L14/THU
L16 1 S L15 AND PRIESTLEY, E?/AU
L17 0 S L16 NOT L5

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=> s l15 and decicco, c?/au

125 DECICCO, C?/AU

L19 1 L15 AND DECICCO, C?/AU

=> s l19 not l16

L20 0 L19 NOT L16

=> s l18 and hydyma, t?/au

0 HYDYMA, T?/AU

L21 0 L18 AND HYDYMA, T?/AU

=> s l18 and zheng, x?/au

3518 ZHENG, X?/AU

L22 0 L18 AND ZHENG, X?/AU

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L18 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2003:970508 HCAPLUS

DOCUMENT NUMBER: 140:174511

TITLE: Mechanism of action and antiviral activity of benzimidazole-based allosteric inhibitors of the hepatitis C virus RNA-dependent RNA polymerase

AUTHOR(S): Tomei, Licia; Altamura, Sergio; Bartholomew, Linda; Biroccio, Antonino; Ceccacci, Alessandra; Pacini, Laura; Narjes, Frank; Gennari, Nadia; Bisbocci, Monica; Incitti, Ilario; Orsatti, Laura; Harper, Steven; Stansfield, Ian; Rowley, Michael; De Francesco, Raffaele; Migliaccio, Giovanni

CORPORATE SOURCE: Istituto di Ricerche di Biologia Molecolare "P. Angeletti", Pomezia-Rome, 00040, Italy

SOURCE: Journal of Virology (2003), 77(24), 13225-13231
CODEN: JOVIAM; ISSN: 0022-538X

PUBLISHER: American Society for Microbiology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The RNA-dependent RNA polymerase of hepatitis C virus (HCV) is the catalytic subunit of the viral RNA amplification machinery and is an appealing target for the development of new therapeutic agents against HCV infection. Nonnucleoside inhibitors based on a benzimidazole scaffold have been recently reported. Compds. of this class are efficient inhibitors of HCV RNA replication in cell culture, thus providing attractive candidates for further development. Here we report the detailed anal. of the mechanism of action of selected benzimidazole inhibitors. Kinetic data and binding expts. indicated that these compds. act as allosteric inhibitors that block the activity of the polymerase prior to the elongation step. Escape mutations that confer resistance to these compds. map to proline 495, a residue located on the surface of the polymerase thumb domain and away from the active site. Substitution of this residue is sufficient to make the HCV enzyme and replicons resistant to the inhibitors. Interestingly, proline 495 lies in a recently identified noncatalytic GTP-binding site, thus validating it as a potential allosteric site that can be targeted by small-mol. inhibitors of HCV polymerase.

IT **658693-60-8**

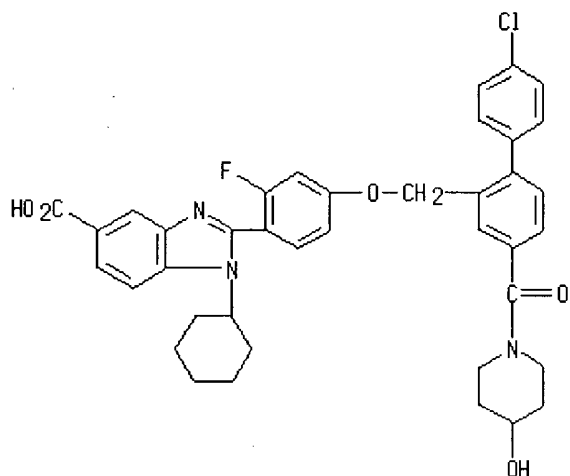
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity);

THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(mechanism of action and antiviral activity of benzimidazole-based allosteric inhibitors of hepatitis C virus RNA-dependent RNA polymerase)

RN **658693-60-8** HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-[[4'-chloro-4-[(4-hydroxy-1-piperidinyl)carbonyl][1,1'-biphenyl]-2-yl]methoxy]-2-fluorophenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing
References

ACCESSION NUMBER: 2003:203407 HCAPLUS
DOCUMENT NUMBER: 138:238181
TITLE: Preparation of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C
INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito
PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
SOURCE: U.S. Pat. Appl. Publ., 406 pp., Cont.-in-part of Appl. No. PCT/JP00/09181.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003050320	A1	20030313	US 2001-939374	20010824
WO 2001047883	A1	20010705	WO 2000-JP9181	20001222
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
JP 2001247550	A2	20010911	JP 2000-391904	20001225
PRIORITY APPLN. INFO.:				
			JP 1999-369008	A 19991227
			WO 2000-JP9181	A2 20001222
			JP 2000-391904	A 20001225
			JP 2001-193786	A 20010626

OTHER SOURCE(S): MARPAT 138:238181
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

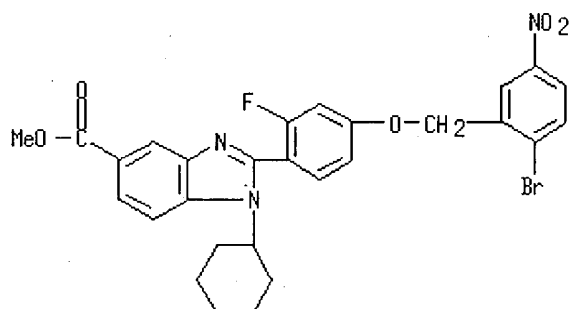
AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, S, CR7, etc.; R1-R4 = H, NO₂, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = Ph, cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, CN, etc.; R7 = H, alkyl] are prepd. and formulated. Compds. I showed HCV polymerase inhibitory activity (data given). E.g., a multi-step synthesis of II.HCl, starting from 2-bromo-5-nitrotoluene and Me 2-(2-fluoro-4-hydroxyphenyl)-1-cyclohexylbenzimidazole-5-carboxylate, was given.

IT 480461-26-5P

RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C)

RN 480461-26-5 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-[(2-bromo-5-nitrophenyl)methoxy]-2-fluorophenyl]-1-cyclohexyl-, methyl ester (9CI) (CA INDEX NAME)



*Good
data*

*Expand to see other
comps.*

Bioscience

L18 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2003:5773 HCAPLUS
DOCUMENT NUMBER: 138:66657
TITLE: Fused cyclic compounds and medicinal use thereof
INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito
PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
SOURCE: PCT Int. Appl., 603 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003000254	A1	20030103	WO 2002-JP6405	20020626
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG,				

US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
 CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

JP 2003212846 A2 20030730 JP 2002-185241 20020625
 BR 2002005684 A 20030617 BR 2002-5684 20020626
 EP 1400241 A1 20040324 EP 2002-743728 20020626

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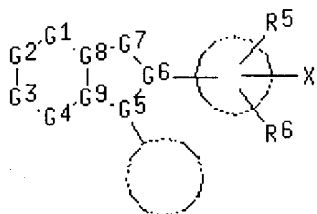
US 2004082635 A1 20040429 US 2003-344997 20030218
 NO 2003000832 A 20030422 NO 2003-832 20030221

PRIORITY APPLN. INFO!

JP 2001-193786 A 20010626
 JP 2001-351537 A 20011116
 WO 2002-JP6405 W 20020626

OTHER SOURCE(S):
 GI

MARPAT 138:66657



AB Fused cyclic compds. represented by the following general formula [I] or pharmaceutically acceptable salts thereof and remedies for hepatitis C contg. these compds.: I wherein each symbol is as defined in the description. Because of having an effect against hepatitis C virus (HVC) based on an HCV polymerase inhibitory effect, these compds. are useful as remedies or preventives for hepatitis C.

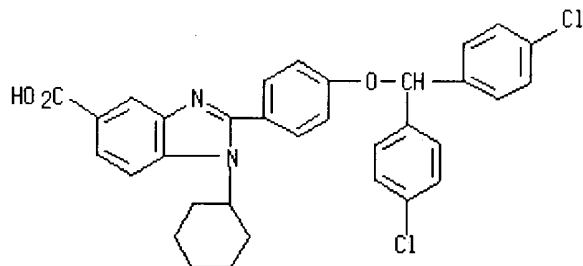
IT 347166-38-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(fused cyclic compds. as hepatitis C virus polymerase inhibitors and antiviral agents)

RN 347166-38-5 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-[bis(4-chlorophenyl)methoxy]phenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

27

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

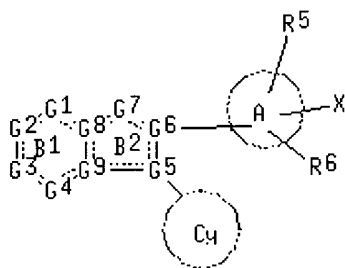
L18 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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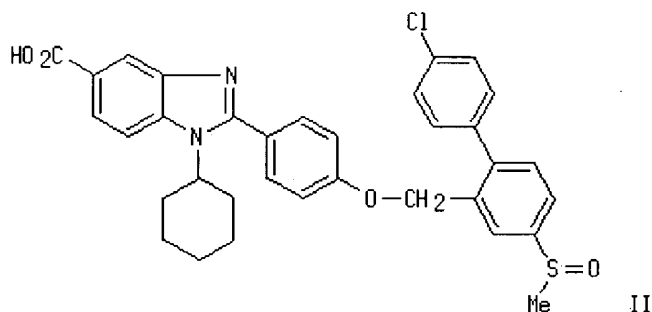
ACCESSION NUMBER: 2001:489367 HCAPLUS
 DOCUMENT NUMBER: 135:76874
 TITLE: Preparation of heterocyclic compounds as remedies for hepatitis C
 INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito
 PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
 SOURCE: PCT Int. Appl., 438 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001047883	A1	20010705	WO 2000-JP9181	20001222
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EP 1162196	A1	20011212	EP 2000-987728	20001222
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000008525	A	20020102	BR 2000-8525	20001222
TR 200103147	T1	20020621	TR 2001-200103147	20001222
NZ 514403	A	20021025	NZ 2000-514403	20001222
AU 763356	B2	20030717	AU 2001-24017	20001222
RU 2223761	C2	20040220	RU 2001-126283	20001222
NO 2001004134	A	20011022	NO 2001-4134	20010824
US 2003050320	A1	20030313	US 2001-939374	20010824
ZA 2001007870	A	20020925	ZA 2001-7870	20010928
PRIORITY APPLN. INFO.:				
			JP 1999-369008	A 19991227
			WO 2000-JP9181	W 20001222
			JP 2000-391904	A 20001225
			JP 2001-193786	A 20010626

OTHER SOURCE(S): MARPAT 135:76874
 GI



I



II

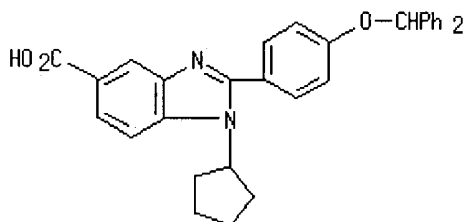
AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2; G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, etc.; R1 - R4 = H, nitro, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = C3-C8 cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, cyano, etc.] are prepd. The benzimidazole deriv. II in vitro showed IC₅₀ of 0.011 μ M against hepatitis C virus polymerase. A formulation is given.

IT **347165-90-6P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of heterocyclic compds. as remedies for hepatitis C)

RN **347165-90-6** HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 1-cyclopentyl-2-[4-(diphenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

27

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
33.22	435.86

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

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ENTRY	SESSION
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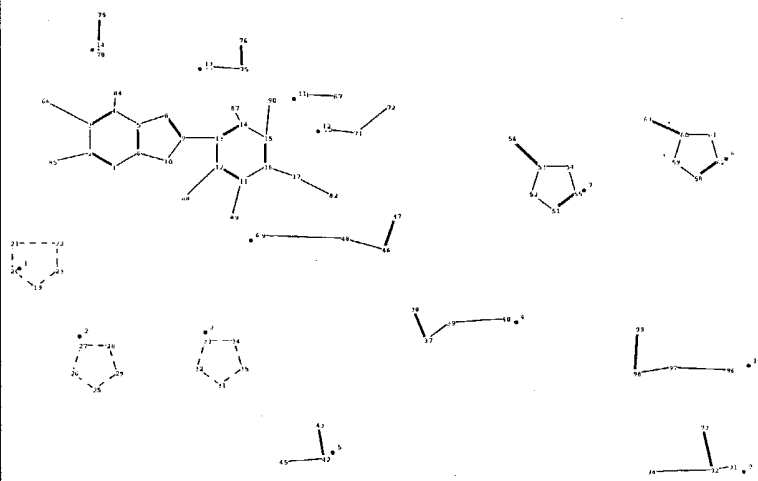
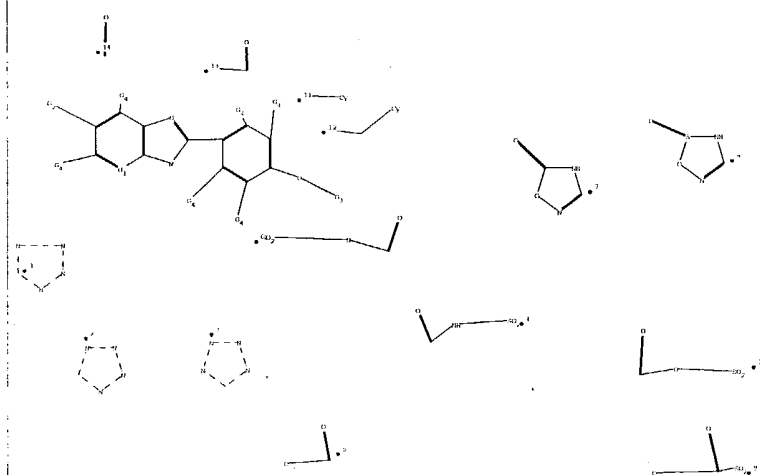
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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY



chain nodes :

17 37 38 39 40 42 43 45 46 47 48 49 56 63 66 67 68 70 71 72 74 75 76
78 79 82 84 85 87 88 89 90 91 92 93 94 96 97 98 99

ring nodes :

1 2 3 4 5 6 8 9 10 11 12 13 14 15 16 19 20 21 22 23 25 26 27 28 29
31 32 33 34 35 51 52 53 54 55 58 59 60 61 62

chain bonds :

2-85 3-66 4-84 9-13 11-89 12-88 14-87 15-90 16-17 17-82 37-38 37-39 39-40
42-43 42-45 46-47 46-48 48-49 53-56 60-63 67-68 70-71 71-72 74-75 75-76 78-79
91-92 92-93 92-94 96-97 97-98 98-99

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-8 6-10 8-9 9-10 11-12 11-16 12-13 13-14 14-15
15-16 19-20 19-23 20-21 21-22 22-23 25-26 25-29 26-27 27-28 28-29 31-32 31-35
32-33 33-34 34-35 51-52 51-55 52-53 53-54 54-55 58-59 58-62 59-60 60-61 61-62

exact/norm bonds :

1-2 1-6 2-3 2-85 3-4 3-66 4-5 4-84 5-6 5-8 6-10 8-9 9-10 9-13 11-89 12-88
14-87 15-90 16-17 17-82 19-20 19-23 20-21 21-22 22-23 25-26 25-29 26-27 27-28
28-29 31-32 31-35 32-33 33-34 34-35 37-38 37-39 39-40 42-43 42-45 46-47 46-48
48-49 51-52 51-55 52-53 53-54 53-56 54-55 58-59 58-62 59-60 60-61 60-63 61-62
67-68 70-71 71-72 74-75 75-76 78-79 91-92 92-93 92-94 96-97 97-98 98-99

normalized bonds :

11-12 11-16 12-13 13-14 14-15 15-16

isolated ring systems :

containing 1 : 11 : 51 : 58 :

G1:C,N

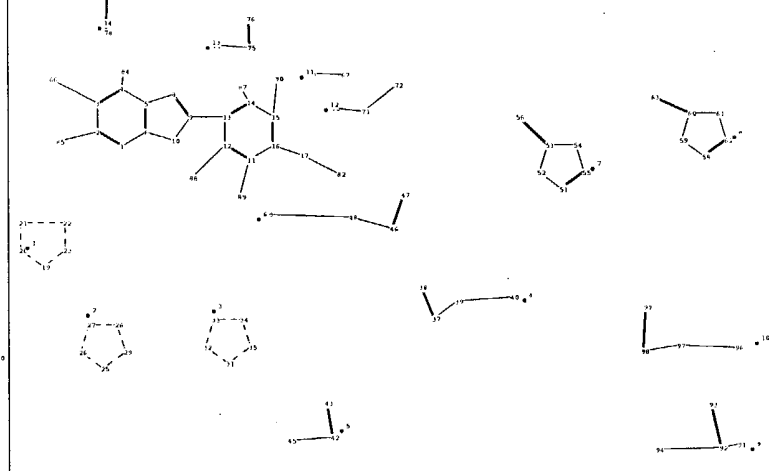
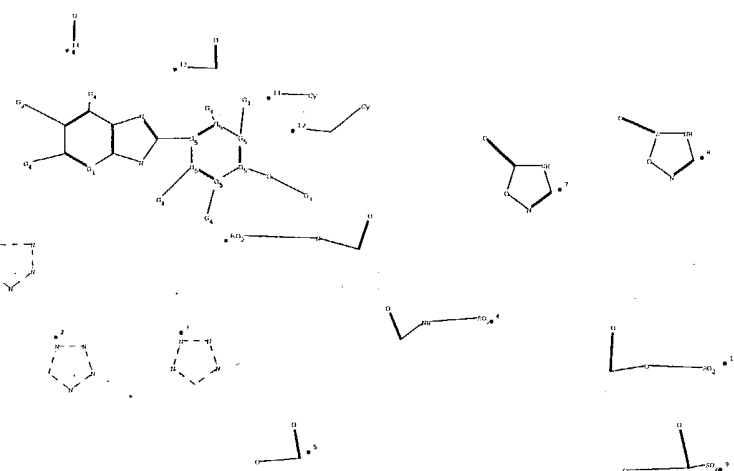
G2:[*1],[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10]

G3:cy,[*11],[*12],[*13],[*14]

G4:H,F,CH3,NH2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom
37:CLASS 38:CLASS 39:CLASS 40:CLASS 42:CLASS 43:CLASS 45:CLASS 46:CLASS 47:CLASS
48:CLASS 49:CLASS 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:CLASS 58:Atom 59:Atom
60:Atom 61:Atom 62:Atom 63:CLASS 66:CLASS 67:Atom 68:CLASS 70:CLASS 71:CLASS
72:Atom 74:CLASS 75:CLASS 76:CLASS 78:CLASS 79:CLASS 82:CLASS 84:CLASS 85:CLASS
87:CLASS 88:CLASS 89:CLASS 90:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS 96:CLASS
97:CLASS 98:CLASS 99:CLASS



main nodes :
 17 37 38 39 40 42 43 45 46 47 48 49 56 63 66 67 68 70 71 72 74 75 76
 78 79 82 84 85 87 88 89 90 91 92 93 94 96 97 98 99

ing nodes :
 1 2 3 4 5 6 8 9 10 11 12 13 14 15 16 19 20 21 22 23 25 26 27 28 29
 31 32 33 34 35 51 52 53 54 55 58 59 60 61 62

main bonds :
 2-85 3-66 4-84 9-13 11-89 12-88 14-87 15-90 16-17 17-82 37-38 37-39 39-40
 42-43 42-45 46-47 46-48 48-49 53-56 60-63 67-68 70-71 71-72 74-75 75-76 78-79
 91-92 92-93 92-94 96-97 97-98 98-99

ing bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 5-8 6-10 8-9 9-10 11-12 11-16 12-13 13-14 14-15
 15-16 19-20 19-23 20-21 21-22 22-23 25-26 25-29 26-27 27-28 28-29 31-32 31-35
 32-33 33-34 34-35 51-52 51-55 52-53 53-54 54-55 58-59 58-62 59-60 60-61 61-62

exact/norm bonds :
 1-2 1-6 2-3 2-85 3-4 3-66 4-5 4-84 5-6 5-8 6-10 8-9 9-10 9-13 11-12 11-16
 11-89 12-13 12-88 13-14 14-15 14-87 15-16 15-90 16-17 17-82 19-20 19-23 20-21
 21-22 22-23 25-26 25-29 26-27 27-28 28-29 31-32 31-35 32-33 33-34 34-35 37-38
 37-39 39-40 42-43 42-45 46-47 46-48 48-49 51-52 51-55 52-53 53-54 53-56 54-55
 58-59 58-62 59-60 60-61 60-63 61-62 67-68 70-71 71-72 74-75 75-76 78-79 91-92
 92-93 92-94 96-97 97-98 98-99

isolated ring systems :
 containing 1 : 11 : 51 : 58 :

1:C,N
 2:[*1],[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10]
 3:cy,[*11],[*12],[*13],[*14]
 4:H,F,CH3,NH2
 5:C,N

ch level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom
37:CLASS 38:CLASS 39:CLASS 40:CLASS 42:CLASS 43:CLASS 45:CLASS 46:CLASS 47:CLASS
48:CLASS 49:CLASS 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:CLASS 58:Atom 59:Atom
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72:Atom 74:CLASS 75:CLASS 76:CLASS 78:CLASS 79:CLASS 82:CLASS 84:CLASS 85:CLASS
87:CLASS 88:CLASS 89:CLASS 90:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS 96:CLASS
97:CLASS 98:CLASS 99:CLASS

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 NEWS 3 JAN 27 Source of Registration (SR) information in REGISTRY updated
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 NEWS 4 JAN 27 A new search aid, the Company Name Thesaurus, available in
 CA/CAPLUS
 NEWS 5 FEB 05 German (DE) application and patent publication number format
 changes
 NEWS 6 MAR 03 MEDLINE and LMedLINE reloaded
 NEWS 7 MAR 03 MEDLINE file segment of TOXCENTER reloaded
 NEWS 8 MAR 03 FRANCEPAT now available on STN
 NEWS 9 MAR 29 Pharmaceutical Substances (PS) now available on STN
 NEWS 10 MAR 29 WPIFV now available on STN
 NEWS 11 MAR 29 New monthly current-awareness alert (SDI) frequency in RAPRA
 NEWS 12 APR 26 PROMT: New display field available
 NEWS 13 APR 26 IFIPAT/IFIUDB/IFICDB: New super search and display field
 available
 NEWS 14 APR 26 LITAlert now available on STN
 NEWS 15 APR 27 NLDB: New search and display fields available
 NEWS 16 May 10 PROUSDDR now available on STN
 NEWS 17 May 19 PROUSDDR: One FREE connect hour, per account, in both May
 and June 2004
 NEWS 18 May 12 EXTEND option available in structure searching
 NEWS 19 May 12 Polymer links for the POLYLINK command completed in REGISTRY

NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
 MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
 AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004

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 DICTIONARY FILE UPDATES: 11 MAY 2004 HIGHEST RN 681211-23-4

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 information enter HELP PROP at an arrow prompt in the file or refer
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<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

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C4 91

C 89 N 90

65
O
||
C
64

G4 67
||

55 G2

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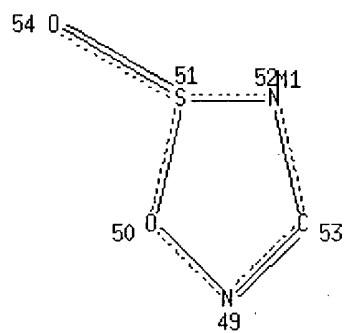
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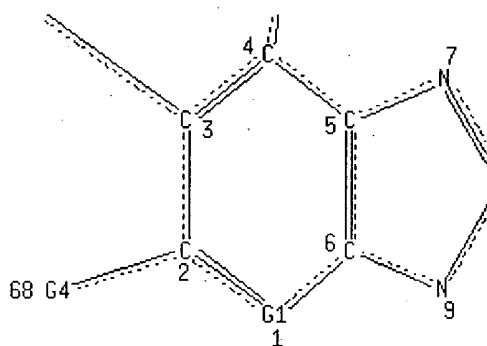
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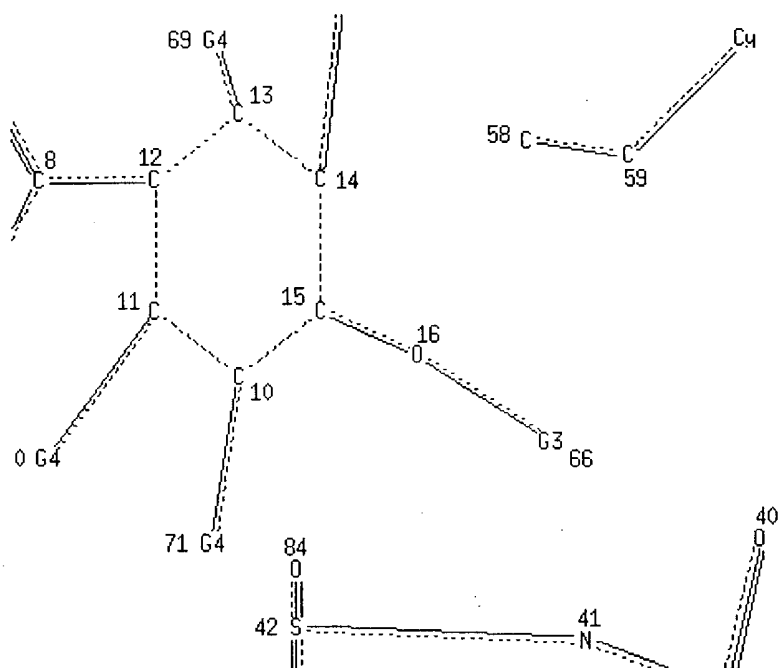


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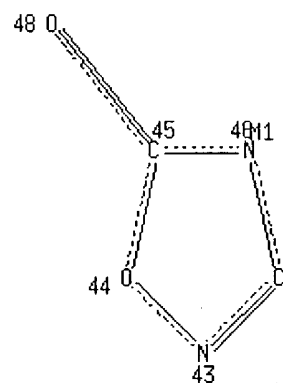


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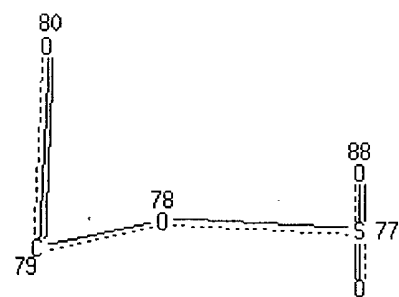
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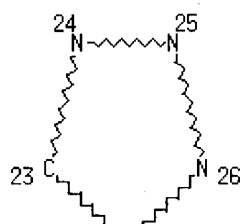
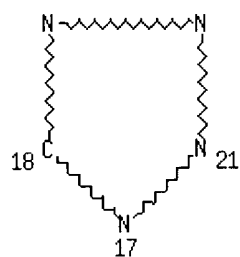
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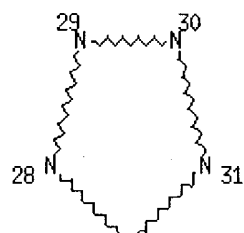
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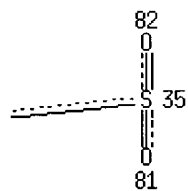
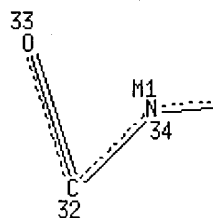
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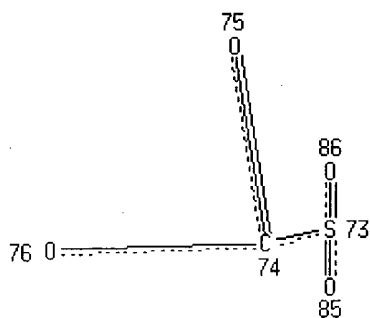
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Page 3-E

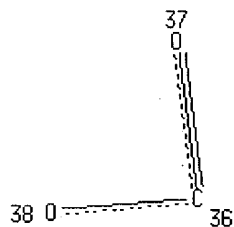


Page 3-F



22

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VAR G1=89/90
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VAR G3=91/57/58/61/64
VAR G4=92/93/94/95
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RSPEC 10 8 43 49
 NUMBER OF NODES IS 95

STEREO ATTRIBUTES: NONE

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 SAMPLE SCREEN SEARCH COMPLETED - 302 TO ITERATE

100.0% PROCESSED 302 ITERATIONS 37 ANSWERS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 4998 TO 7082
 PROJECTED ANSWERS: 376 TO 1104

L2 37 SEA SSS SAM L1

=> s 11 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
 FULL SEARCH INITIATED 15:56:16 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 6058 TO ITERATE

100.0% PROCESSED 6058 ITERATIONS 599 ANSWERS
 SEARCH TIME: 00.00.02

L3 599 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	156.26	156.47

FILE 'HCAPLUS' ENTERED AT 15:56:23 ON 12 MAY 2004
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FILE COVERS 1907 - 12 May 2004 VOL 140 ISS 20
 FILE LAST UPDATED: 11 May 2004 (20040511/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13
 L4 14 L3

=> s 14 and beaulieu, p?
 50 BEAULIEU

TERM 'P?' EXCEEDED TRUNCATION LIMITS - SEARCH ENDED

You have entered a truncated stem which occurs in too many terms. Make the stem longer and try again. For example, if your original term was 'degr?' to search for variations and the abbreviation for 'degradation', you could replace it with the expression '(degrdn OR degrad?)'. If your search term was numeric, e.g., 'C>5', reduce the size of the range.

=> s 14 and beaulieu, p?/au
 120 BEAULIEU, P?/AU
 L5 2 L4 AND BEAULIEU, P?/AU

=> d 15, ibib abs fhitr, 1-2

L5 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
 Text References

ACCESSION NUMBER: 2003:981461 HCAPLUS
 DOCUMENT NUMBER: 140:246106
 TITLE: Non-nucleoside inhibitors of the hepatitis C virus NS5B polymerase: discovery and preliminary SAR of benzimidazole derivatives
 AUTHOR(S): Beaulieu, Pierre L.; Bos, Michael; Bousquet, Yves; Fazal, Gulrez; Gauthier, Jean; Gillard, James; Goulet, Sylvie; LaPlante, Steven; Poupart, Marc-Andre; Lefebvre, Sylvain; McKercher, Ginette; Pellerin, Charles; Austel, Volkhard; Kukolj, George
 CORPORATE SOURCE: Department of Chemistry, Research and Development, Boehringer Ingelheim (Canada) Ltd., Laval, QC, H7S 2G5, Can.
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(1), 119-124
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Benzimidazole 5-carboxamide derivs. from a combinatorial screening library were discovered as specific inhibitors of the NS5B polymerase of the hepatitis C virus (HCV). Initial hit-to-lead activities taking advantage of high-throughput parallel synthetic techniques, identified a 1,2-disubstituted benzimidazole 5-carboxylic acid scaffold as the min. core for biol. activity. Potent analogs in this series inhibit the polymerase at low micromolar concns. and provide an attractive 'drug-like' lead structure for further optimization and the development of potential HCV therapeutics.

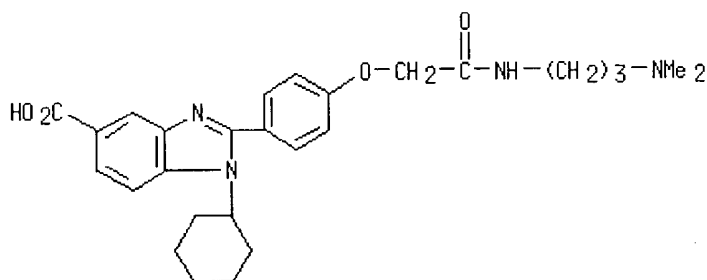
IT 390815-16-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(discovery and preliminary SAR of benzimidazole derivs. as inhibitors of hepatitis C virus NS5B polymerase)

RN 390815-16-4 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[4-[2-[[3-(dimethylamino)propyl]amino]-2-oxoethoxy]phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2002:51438 HCAPLUS

DOCUMENT NUMBER: 136:118447

TITLE: Preparation of benzimidazolecarboxylates and related compounds as viral polymerase inhibitors

INVENTOR(S): Beaulieu, Pierre Louis; Fazal, Gulrez; Gillard, James; Kukolj, George; Austel, Volkhard

PATENT ASSIGNEE(S): Boehringer Ingelheim (Canada) Ltd., Can.

SOURCE: PCT Int. Appl., 322 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004425	A2	20020117	WO 2001-CA989	20010704

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 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 2002065418 A1 20020530 US 2001-898297 20010703

US 6448281 B2 20020910

EP 1301487 A2 20030416 EP 2001-951274 20010704

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JP 2004502761 T2 20040129 JP 2002-509292 20010704

US 6479508 B1 20021112 US 2001-995099 20011127

WO 2002070739 A2 20020912 WO 2002-CA323 20020306

WO 2002070739 A3 20030530

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EP 1370682 A2 20031217 EP 2002-712681 20020306

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US 2003232816 A1 20031218 US 2002-238282 20020910

PRIORITY APPLN. INFO.:

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US 2001-274374P P 20010308

US 2001-281343P P 20010405

US 2001-898297 A3 20010703

WO 2001-CA989 W 20010704

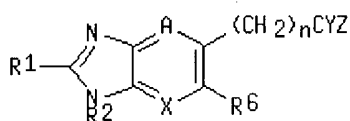
US 2001-995099 A3 20011127

WO 2002-CA323 W 20020306

OTHER SOURCE(S):

MARPAT 136:118447

GI



I

AB Title compds. [I; X = CH, N; Y = O, S; Z = OH, NH₂, NMe₃, NHR₃, OR₃, 5-6
 membered (substituted) heterocyclyl; A = N, COR₇, CR₅; R₅ = H, halo,
 alkyl; R₇ = H, alkyl; X and A are not both N; R₆ = H, halo, alkyl, OR₇; R₇
 = H, alkyl; R₁ = (substituted) hetero(bi)cyclyl, Ph, phenylalkyl,
 alkenyl, phenylalkenyl, cycloalkyl, alkyl, CF₃; R₂ = (substituted) alkyl,
 cycloalkyl, cycloalkylalkyl, bicycloalkyl, adamantyl, Ph, pyridyl; R₃ = H,
 alkyl, cycloalkyl, cycloalkylalkyl, aryl, arylalkyl, alkenyl,
 cycloalkylalkenyl, arylalkenyl, dialkylamino, heterocyclyl, etc.; n = 0,
 1], were prep'd. Thus, Me 3-amino-4-cyclohexylaminobenzoate (prepn.
 given), 2-pyridinecarboxaldehyde, and Oxone were stirred in DMF to give
 80% Et 1-cyclohexyl-2-pyridin-2-yl-1H-benzimidazole-5-carboxylate, which
 was sapon'd. with aq. NaOH in MeOH to give 91% 1-cyclohexyl-2-pyridin-2-yl-
 1H-benzimidazole-5-carboxylic acid. The latter inhibited hepatitis C
 virus RNA dependent polymerase (NS5B) with IC₅₀ = 1-5 μ M.

IT 347166-09-0P

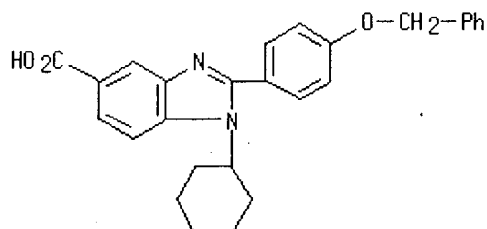
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzimidazolecarboxylates and related compds. as viral polymerase inhibitors)

RN 347166-09-0 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)



=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	16.59	173.06
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.39	-1.39

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 MAY 2004 HIGHEST RN 681211-23-4
 DICTIONARY FILE UPDATES: 11 MAY 2004 HIGHEST RN 681211-23-4

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L6 STRUCTURE UPLOADED

=> 16

L6 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

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L6 HAS NO ANSWERS

L6 STR

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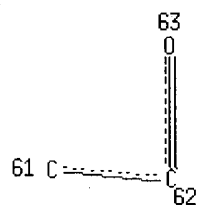
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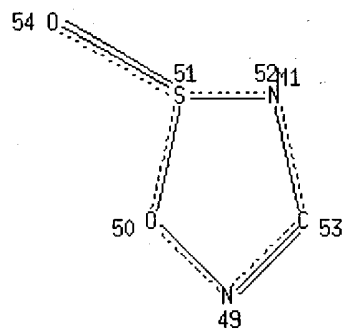
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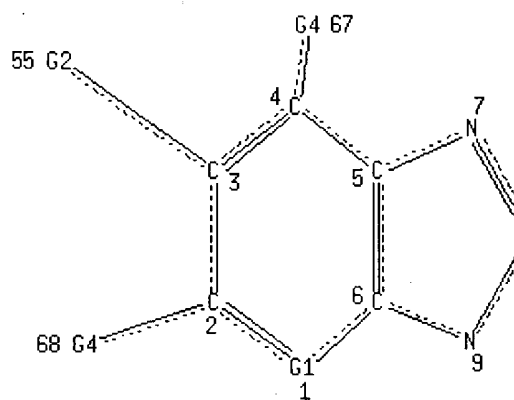
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Page 2-A

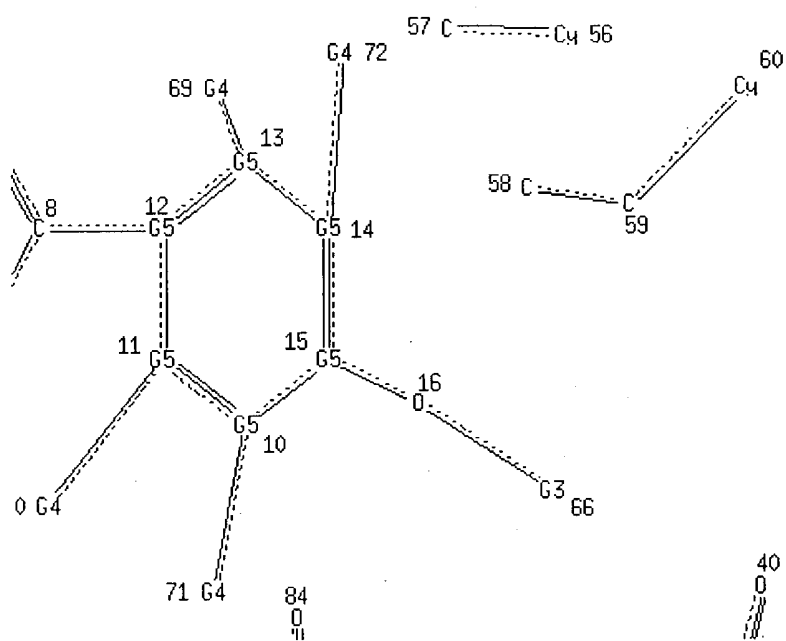


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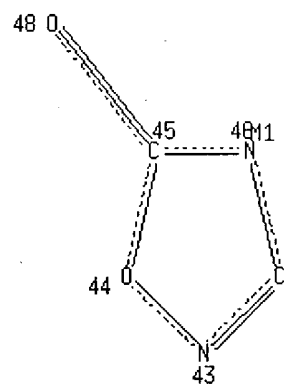


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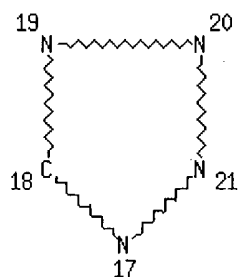
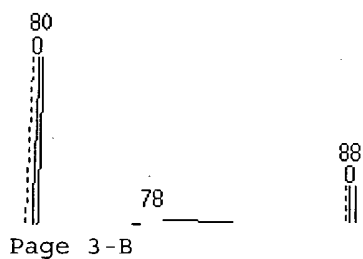
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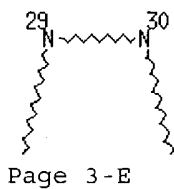
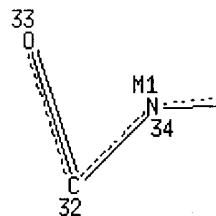
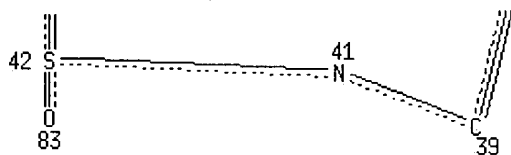
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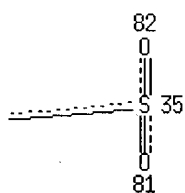


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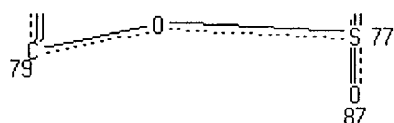


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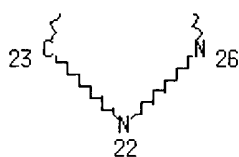




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Page 4-B



Page 4-D



Page 4-E

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 VAR G4=92/93/94/95
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DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 16 32 33 34 35 36 37 38 39 40 41 42 48 54 57 58 59
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 10 8 43 49

NUMBER OF NODES IS 97

STEREO ATTRIBUTES: NONE

=> s 16

SAMPLE SEARCH INITIATED 16:00:40 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 2049 TO ITERATE

48.8% PROCESSED 1000 ITERATIONS

19 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 38265 TO 43695

PROJECTED ANSWERS: 404 TO 1152

L7 19 SEA SSS SAM L6

=> s 16 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 16:00:48 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 40648 TO ITERATE

100.0% PROCESSED 40648 ITERATIONS
SEARCH TIME: 00.00.02

599 ANSWERS

L8 599 SEA SSS FUL L6

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	170.54	343.60
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-1.39

FILE 'HCAPLUS' ENTERED AT 16:20:18 ON 12 MAY 2004
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FILE COVERS 1907 - 12 May 2004 VOL 140 ISS 20
FILE LAST UPDATED: 11 May 2004 (20040511/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 18/thu

14 L8
591965 THU/RL
L9 8 L8/THU
(L8 (L) THU/RL)

=> d 19, ibib abs fhitr, 1-8

L9 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2003:981461 HCAPLUS
DOCUMENT NUMBER: 140:246106
TITLE: Non-nucleoside inhibitors of the hepatitis C virus NS5B polymerase: discovery and preliminary SAR of benzimidazole derivatives
AUTHOR(S): Beaulieu, Pierre L.; Bos, Michael; Bousquet, Yves;

Fazal, Gulrez; Gauthier, Jean; Gillard, James; Goulet, Sylvie; LaPlante, Steven; Poupart, Marc-Andre; Lefebvre, Sylvain; McKercher, Ginette; Pellerin, Charles; Austel, Volkhard; Kukolj, George
 CORPORATE SOURCE: Department of Chemistry, Research and Development, Boehringer Ingelheim (Canada) Ltd., Laval, QC, H7S 2G5, Can.
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(1), 119-124
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

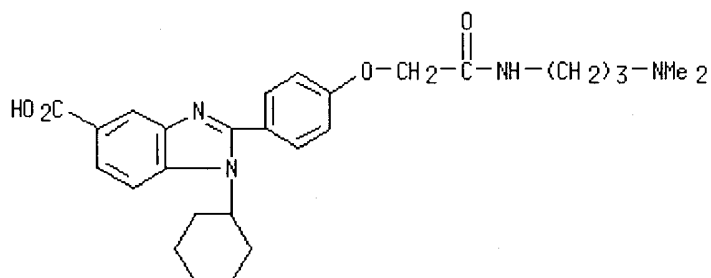
AB Benzimidazole 5-carboxamide derivs. from a combinatorial screening library were discovered as specific inhibitors of the NS5B polymerase of the hepatitis C virus (HCV). Initial hit-to-lead activities taking advantage of high-throughput parallel synthetic techniques, identified a 1,2-disubstituted benzimidazole 5-carboxylic acid scaffold as the min. core for biol. activity. Potent analogs in this series inhibit the polymerase at low micromolar concns. and provide an attractive 'drug-like' lead structure for further optimization and the development of potential HCV therapeutics.

IT 390815-16-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (discovery and preliminary SAR of benzimidazole derivs. as inhibitors of hepatitis C virus NS5B polymerase)

RN 390815-16-4 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[4-[2-[[3-(dimethylamino)propyl]amino]-2-oxoethoxy]phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2003:970508 HCAPLUS

DOCUMENT NUMBER: 140:174511

TITLE: Mechanism of action and antiviral activity of benzimidazole-based allosteric inhibitors of the hepatitis C virus RNA-dependent RNA polymerase

AUTHOR(S): Tomei, Licia; Altamura, Sergio; Bartholomew, Linda; Biroccio, Antonino; Ceccacci, Alessandra; Pacini, Laura; Narjes, Frank; Gennari, Nadia; Bisbocci, Monica; Incitti, Ilario; Orsatti, Laura; Harper, Steven; Stansfield, Ian; Rowley, Michael; De Francesco, Raffaele; Migliaccio, Giovanni

CORPORATE SOURCE: Istituto di Ricerche di Biologia Molecolare "P. Angeletti", Pomezia-Rome, 00040, Italy
 SOURCE: Journal of Virology (2003), 77(24), 13225-13231
 CODEN: JOVIAM; ISSN: 0022-538X
 PUBLISHER: American Society for Microbiology
 DOCUMENT TYPE: Journal
 LANGUAGE: English

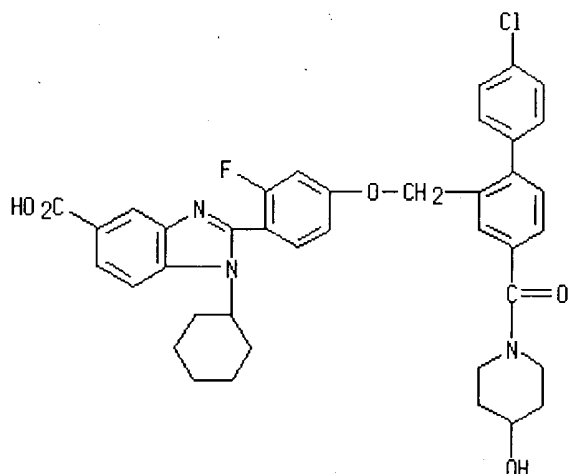
AB The RNA-dependent RNA polymerase of hepatitis C virus (HCV) is the catalytic subunit of the viral RNA amplification machinery and is an appealing target for the development of new therapeutic agents against HCV infection. Nonnucleoside inhibitors based on a benzimidazole scaffold have been recently reported. Compds. of this class are efficient inhibitors of HCV RNA replication in cell culture, thus providing attractive candidates for further development. Here we report the detailed anal. of the mechanism of action of selected benzimidazole inhibitors. Kinetic data and binding expts. indicated that these compds. act as allosteric inhibitors that block the activity of the polymerase prior to the elongation step. Escape mutations that confer resistance to these compds. map to proline 495, a residue located on the surface of the polymerase thumb domain and away from the active site. Substitution of this residue is sufficient to make the HCV enzyme and replicons resistant to the inhibitors. Interestingly, proline 495 lies in a recently identified noncatalytic GTP-binding site, thus validating it as a potential allosteric site that can be targeted by small-mol. inhibitors of HCV polymerase.

IT 658693-60-8

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (mechanism of action and antiviral activity of benzimidazole-based allosteric inhibitors of hepatitis C virus RNA-dependent RNA polymerase)

RN 658693-60-8 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-[[4'-chloro-4-[(4-hydroxy-1-piperidinyl)carbonyl][1,1'-biphenyl]-2-yl]methoxy]-2-fluorophenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

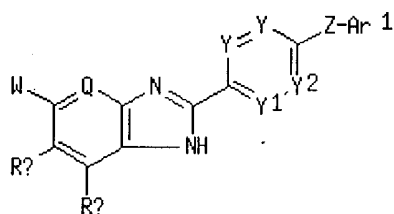
Full Text Citing References

ACCESSION NUMBER: 2003:319709 HCAPLUS

DOCUMENT NUMBER: 138:338144
 TITLE: Preparation of 2-phenyl benzimidazoles and imidazo-[4,5]pyridines as Cds1/Chk2-inhibitors and adjuvants to chemotherapy or radiation therapy in the treatment of cancer
 INVENTOR(S): Arienti, Kristen L.; Axe, Frank U.; Breitenbucher, J. Guy; Huang, Liming; Lee, Alice; McClure, Kelly J.
 PATENT ASSIGNEE(S): Ortho-McNeil Pharmaceutical, Inc., USA
 SOURCE: PCT Int. Appl., 144 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003032984	A1	20030424	WO 2002-US33371	20021018
WO 2003032984	C1	20031120		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003176438	A1	20030918	US 2002-273487	20021018
NO 2003002759	A	20030818	NO 2003-2759	20030617
PRIORITY APPLN. INFO.:				
			US 2001-330304P	P 20011019
			WO 2002-US33371	W 20021018

OTHER SOURCE(S): MARPAT 138:338144
 GI



AB 2-Aryl-substituted benzimidazoles and imidazo[4,5]pyridines (shown as I; e.g. 2-[4-(4-chlorophenoxy)phenyl]-1H-benzimidazole-5-carboxylic acid amide (II)) are disclosed as inhibitors of Cds1 and useful as adjuvants to chemotherapy or radiation therapy in the treatment of cancer. For I: W is COOH, -C(O)NHR1, or -SO2NHR1 (R1 is H or C1-4alkyl); Q is N or CH; Ra and Rb are H or halogen; Y, Y1 and Y2 = N and C-Rc with the proviso that 0, 1 or 2 of Y, Y1 and Y2 are N and at least 2 of Rc must be H; Rc = -H, -OH, -C1-6alkyl, -SCF3, halo, -CF3 and -OCF3; Z = O, S, SO, SO2, SO2NR2, NR2SO2, NH, CONR2, piperazinediyl or a covalent bond; R2 is H or C1-4alkyl; Ar1 is an arom. group as defined in the claims. IC50 values are reported for inhibition of human Cds1 checkpoint kinase by 103 examples of I, e.g. 3 nM for 2-[4-(4-chloro-3-trifluoromethylphenoxy)phenyl]-1H-benzimidazole-5-carboxylic acid amide.

Addnl. studies were (i) detn. of the effect of II on tumor cell line clonogenic survival, (ii) effect of II on tumor growth in murine xenograft models, (iii) detn. of the effect of 14 examples of I on radiation-induced apoptosis in isolated primary cells, and (iv) detn. of the effect of II on radiation-induced apoptosis in splenocytes in vivo. Although the methods of prepn. are not claimed, ~100 example prepn. are included.

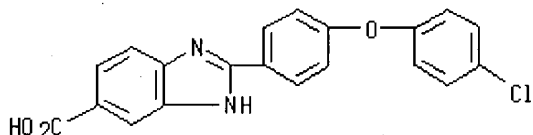
IT 516480-80-1P, 2-[4-(4-Chlorophenoxy)phenyl]-1H-benzimidazole-5-carboxylic acid

RL: PAC (Pharmacological activity); RCT (Reactant); **THU (Therapeutic use); THU (Therapeutic use);** BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; prepn. of benzimidazoles and imidazopyridines as Cds1/Chk2-inhibitors and adjuvants to chemotherapy or radiation therapy in treatment of cancer)

RN 516480-80-1 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(4-chlorophenoxy)phenyl]- (9CI)
(CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2003:261620 HCAPLUS
DOCUMENT NUMBER: 138:287673
TITLE: Preparation of phenylbenzimidazole compounds useful for treating hepatitis C virus
INVENTOR(S): Priestley, Eldon Scott; Decicco, Carl P.; Hudyma, Thomas W.; Zheng, Xiaofan
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003026587	A2	20030403	WO 2002-US30989	20020926
WO 2003026587	A3	20031106		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003134853	A1	20030717	US 2002-259041	20020926

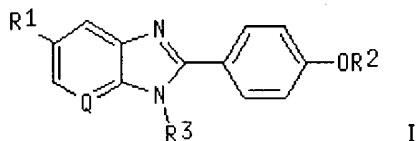
NO

US 2004067976
PRIORITY APPLN. INFO.:

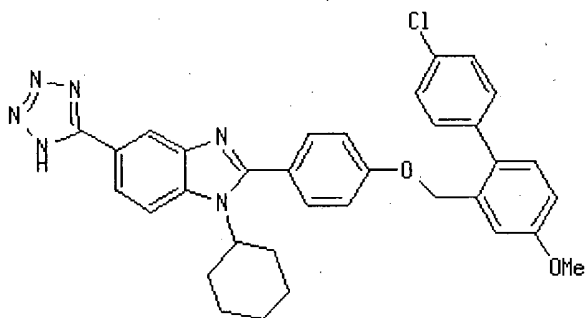
A1 20040408

US 2003-648873 20030827
US 2001-324874P P 20010926
US 2002-259041 B1 20020926

OTHER SOURCE(S): MARPAT 138:287673
GI



I



II

AB Compds. of formula I [Q = CH, N; R1 = tetrazolyl, MeCONHSO2, PhCONHSO2, etc.; R2 = CH2-aryl, CHPh2, etc.; R3 = cycloalkyl] are prepd. which are useful in treating viral hepatitis C. Thus, II was prepd. and had an IC50 of 0.14 μ M against HCV NS5B RdRp (RNA-dependent RNA polymerase).

IT 503857-56-5P

RL: PAC (Pharmacological activity); RCT (Reactant); **THU (Therapeutic use)**; **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of phenylbenzimidazole compds. for treating hepatitis C viral infection)

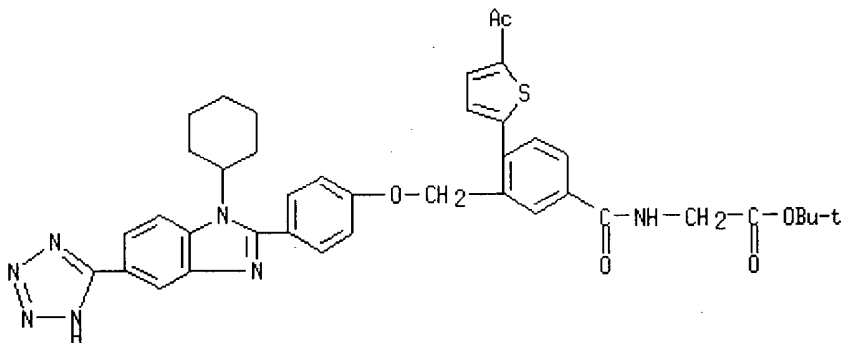
RN 503857-56-5 HCAPLUS

CN Glycine, N-[4-(5-acetyl-2-thienyl)-3-[[4-[1-cyclohexyl-5-(1H-tetrazol-5-yl)-1H-benzimidazol-2-yl]phenoxy]methyl]benzoyl]-, 1,1-dimethylethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

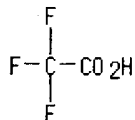
CM 1

CRN 503857-55-4

CMF C40 H41 N7 O5 S



CM 2

CRN 76-05-1
CMF C2 H F3 O2

L9 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2003:203407 HCAPLUS
 DOCUMENT NUMBER: 138:238181
 TITLE: Preparation of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C
 INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito
 PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
 SOURCE: U.S. Pat. Appl. Publ., 406 pp., Cont.-in-part of Appl. No. PCT/JP00/09181.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003050320	A1	20030313	US 2001-939374	20010824
WO 2001047883	A1	20010705	WO 2000-JP9181	20001222
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG JP 2001247550 A2 20010911 JP 2000-391904 20001225				
PRIORITY APPLN. INFO.:			JP 1999-369008 A 19991227	
			WO 2000-JP9181 A2 20001222	
			JP 2000-391904 A 20001225	
			JP 2001-193786 A 20010626	
OTHER SOURCE(S):			MARPAT 138:238181	
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5,

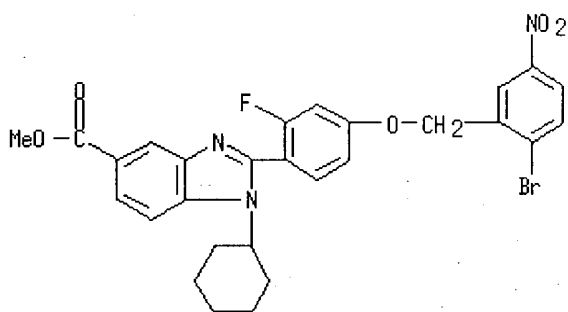
G6, G8, G9 = C, N; G7 = O, S, CR7, etc.; R1-R4 = H, NO₂, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = Ph, cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, CN, etc.; R7 = H, alkyl are prepd. and formulated. Compds. I showed HCV polymerase inhibitory activity (data given). E.g., a multi-step synthesis of II.HCl, starting from 2-bromo-5-nitrotoluene and Me 2-(2-fluoro-4-hydroxyphenyl)-1-cyclohexylbenzimidazole-5-carboxylate, was given.

IT 480461-26-5P

RL: PAC (Pharmacological activity); RCT (Reactant); **THU (Therapeutic use); THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C)

RN 480461-26-5 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-[(2-bromo-5-nitrophenyl)methoxy]-2-fluorophenyl]-1-cyclohexyl-, methyl ester (9CI) (CA INDEX NAME)



Biological

L9 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

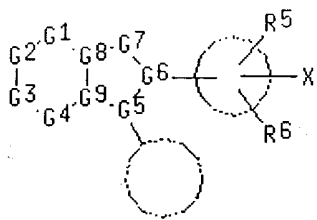
Full Text Citing References

ACCESSION NUMBER: 2003:5773 HCAPLUS
DOCUMENT NUMBER: 138:66657
TITLE: Fused cyclic compounds and medicinal use thereof
INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito
PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
SOURCE: PCT Int. Appl., 603 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003000254	A1	20030103	WO 2002-JP6405	20020626
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
JP 2003212846	A2	20030730	JP 2002-185241	20020625
BR 2002005684	A	20030617	BR 2002-5684	20020626

EP 1400241 A1 20040324 EP 2002-743728 20020626
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
 US 2004082635 A1 20040429 US 2003-344997 20030218
 NO 2003000832 A 20030422 NO 2003-832 20030221
 PRIORITY APPLN. INFO.: JP 2001-193786 A 20010626
 JP 2001-351537 A 20011116
 WO 2002-JP6405 W 20020626

OTHER SOURCE(S): MARPAT 138:66657
 GI



AB Fused cyclic compds. represented by the following general formula [I] or pharmaceutically acceptable salts thereof and remedies for hepatitis C contg. these compds.: I wherein each symbol is as defined in the description. Because of having an effect against hepatitis C virus (HVC) based on an HCV polymerase inhibitory effect, these compds. are useful as remedies or preventives for hepatitis C.

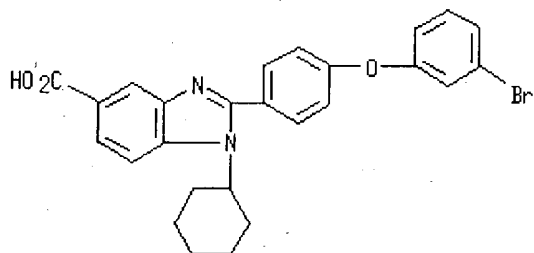
IT 347165-35-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(fused cyclic compds. as hepatitis C virus polymerase inhibitors and antiviral agents)

RN 347165-35-9 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(3-bromophenoxy)phenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2002:51438 HCAPLUS

DOCUMENT NUMBER: 136:118447

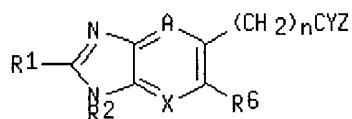
TITLE: Preparation of benzimidazolecarboxylates and related compounds as viral polymerase inhibitors

INVENTOR(S): Beaulieu, Pierre Louis; Fazal, Gulrez; Gillard, James;

PATENT ASSIGNEE(S): Kukolj, George; Austel, Volkhard
 SOURCE: Boehringer Ingelheim (Canada) Ltd., Can.
 PCT Int. Appl., 322 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004425	A2	20020117	WO 2001-CA989	20010704
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002065418	A1	20020530	US 2001-898297	20010703
US 6448281	B2	20020910		
EP 1301487	A2	20030416	EP 2001-951274	20010704
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004502761	T2	20040129	JP 2002-509292	20010704
US 6479508	B1	20021112	US 2001-995099	20011127
WO 2002070739	A2	20020912	WO 2002-CA323	20020306
WO 2002070739	A3	20030530		
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EP 1370682	A2	20031217	EP 2002-712681	20020306
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2003232816	A1	20031218	US 2002-238282	20020910
PRIORITY APPLN. INFO.:				
			US 2000-216084P	P 20000706
			US 2001-274374P	P 20010308
			US 2001-281343P	P 20010405
			US 2001-898297	A3 20010703
			WO 2001-CA989	W 20010704
			US 2001-995099	A3 20011127
			WO 2002-CA323	W 20020306

OTHER SOURCE(S): MARPAT 136:118447
 GI



I

AB Title compds. [I; X = CH, N; Y = O, S; Z = OH, NH₂, NMeR₃, NHR₃, OR₃, 5-6 membered (substituted) heterocyclyl; A = N, COR₇, CR₅; R₅ = H, halo, alkyl; R₇ = H, alkyl; X and A are not both N; R₆ = H, halo, alkyl, OR₇; R₇ = H, alkyl; R₁ = (substituted) hetero(bi)cyclyl, Ph, phenylalkyl, alkenyl, phenylalkenyl, cycloalkyl, alkyl, CF₃; R₂ = (substituted) alkyl, cycloalkyl, cycloalkylalkyl, bicycloalkyl, adamantyl, Ph, pyridyl; R₃ = H, alkyl, cycloalkyl, cycloalkylalkyl, aryl, arylalkyl, alkenyl, cycloalkylalkenyl, arylalkenyl, dialkylamino, heterocyclyl, etc.; n = 0, 1], were prepd. Thus, Me 3-amino-4-cyclohexylaminobenzoate (prepn. given), 2-pyridinecarboxaldehyde, and Oxone were stirred in DMF to give 80% Et 1-cyclohexyl-2-pyridin-2-yl-1H-benzimidazole-5-carboxylate, which was sapond. with aq. NaOH in MeOH to give 91% 1-cyclohexyl-2-pyridin-2-yl-1H-benzimidazole-5-carboxylic acid. The latter inhibited hepatitis C virus RNA dependent polymerase (NS5B) with IC₅₀ = 1-5 μ M.

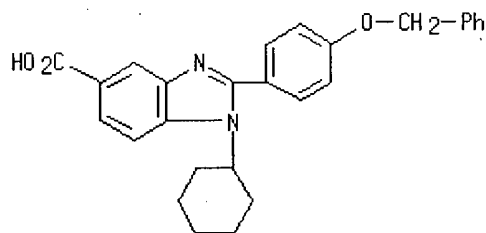
IT **347166-09-0P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); **THU** (**Therapeutic use**); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzimidazolecarboxylates and related compds. as viral polymerase inhibitors)

RN **347166-09-0** HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)



L9 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2001:489367 HCAPLUS
 DOCUMENT NUMBER: 135:76874
 TITLE: Preparation of heterocyclic compounds as remedies for hepatitis C
 INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, Atsuhito
 PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
 SOURCE: PCT Int. Appl., 438 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001047883	A1	20010705	WO 2000-JP9181	20001222
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 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

EP 1162196 A1 20011212 EP 2000-987728 20001222

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO

BR 2000008525 A 20020102 BR 2000-8525 20001222

TR 200103147 T1 20020621 TR 2001-200103147 20001222

NZ 514403 A 20021025 NZ 2000-514403 20001222

AU 763356 B2 20030717 AU 2001-24017 20001222

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NO 2001004134 A 20011022 NO 2001-4134 20010824

US 2003050320 A1 20030313 US 2001-939374 20010824

ZA 2001007870 A 20020925 ZA 2001-7870 20010928

PRIORITY APPLN. INFO.:

JP 1999-369008 A 19991227

WO 2000-JP9181 W 20001222

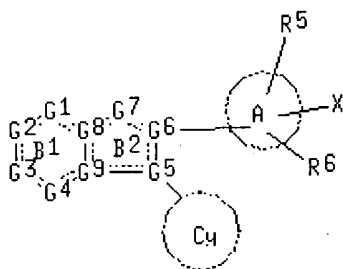
JP 2000-391904 A 20001225

JP 2001-193786 A 20010626

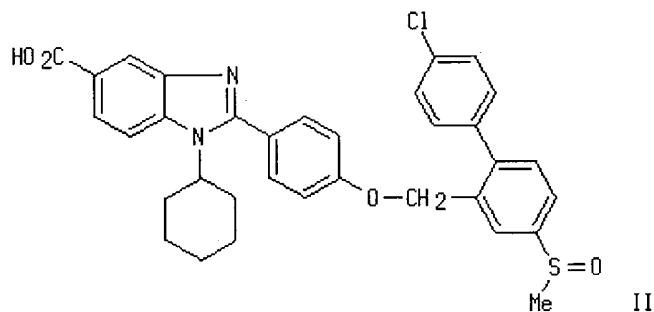
OTHER SOURCE(S):

MARPAT 135:76874

GI



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II

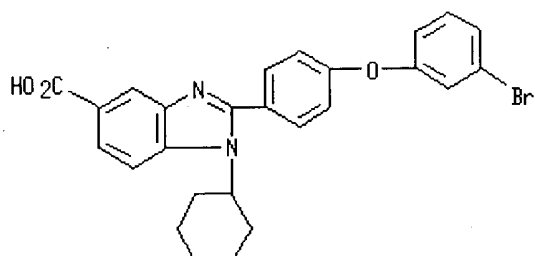
AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2; G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, etc.; R1 - R4 = H, nitro, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = C3-C8 cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, cyano, etc.] are prepd. The benzimidazole deriv. II in vitro showed IC50 of 0.011 μ M against hepatitis C virus polymerase. A formulation is given.

IT 347165-35-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of heterocyclic compds. as remedies for hepatitis C)

RN 347165-35-9 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(3-bromophenoxy)phenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L3 599 S L1 FULL

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L6 STRUCTURE UPLOADED

L7 19 S L6

L8 599 S L6 FULL

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